

A HYBRID COLLOCATION-PERTURBATION APPROACH FOR PDES WITH RANDOM DOMAINS

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ABSTRACT. In this work we consider the problem of approximating the statistics of a given Quantity of Interest (QoI) that depends on the solution of a linear elliptic PDE defined over a random domain parameterized by N random variables. The random domain is split into large and small variations contributions. The large variations are approximated by applying a sparse grid stochastic collocation method. The small variations are approximated with a stochastic collocation-perturbation method. Convergence rates for the variance of the QoI are derived and compared to those obtained in numerical experiments. Our approach significantly reduces the dimensionality of the stochastic problem. The computational cost of this method increases at most quadratically with respect to the number of dimensions of the small variations. Moreover, for the case that the small and large variations are independent the cost increases linearly.

1. INTRODUCTION

The problem of design under the uncertainty of the underlying domain can be encountered in many real life applications. For example, in semiconductor fabrication the underlying geometry becomes increasingly uncertain as the physical scales are reduced [24]. This uncertainty is propagated to an important Quantity of Interest (QoI) of the semiconductor circuit. If the variance of the capacitance is high this could lead to low yields during the manufacturing process. It is important to quantify the uncertainty of the QoI in the circuit to be able to maximize yields. This will have a direct impact in reducing the costly and time-consuming design cycle. Other examples included graphene nano-sheet fabrication [12]. In this paper we focus on the problem of how to efficiently compute the statistics of the QoI given uncertainty in the underlying geometry.

Uncertainty Quantification (UQ) methods applied to Partial Differential Equations (PDEs) with random geometries can be mostly divided into collocation and perturbation approaches. For large deviations of the geometry the collocation method [4, 7, 23, 5] is well suited. In addition, in [5, 10] the authors derive error estimates of the solution with respect to the number of stochastic variables in the geometry description. However, this approach is effective for a moderate number of stochastic variables. In contrast, the perturbation approaches introduced in [11, 24] are efficient for high dimensional small perturbations of the domain.

We represent the domain in terms of a series of random variables and then remap the corresponding PDE to a deterministic domain with random coefficients. The

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random geometry is split into small and large deviations. A collocation sparse grid method is used to approximate the contribution to the QoI from the first large deviations N_s terms of the stochastic domain expansion. Conversely, the contribution of the small deviations (the tail) are cheaply computed with a collocation and perturbation method.

We derive rigorous convergence analysis of the statistics of the QoI in terms of the number of collocation points and the perturbation approximation of the tail. Analytic estimates show that the error of the QoI for the hybrid collocation-perturbation method (or the hybrid perturbation method for short) decays quadratically with respect to the of sum of the series coefficients of the series expansion of the tail. This is in contrast to the linear decay of the error estimates derived in [5] for the pure stochastic collocation approach. Furthermore, numerical experiments show faster convergence than the stochastic collocation approach.

The outline of the paper is the following: In Section 2 mathematical background material is introduced. In Section 3 we set up the problem and reformulate the random domain elliptic PDE problem onto a deterministic domain with random matrix coefficients. We assume that the random boundary is parameterized by N random variables. In section 4 we derive the hybrid collocation-perturbation approach. The approach reduces to computing *mean* and *variance correction* terms that quantifies the contribution from the tail of the random domain expansion. In Section 5 we show that the mean and variance correction terms can be analytically extended onto a well defined region in \mathbb{C}^{N_s} . In Section 6 we derive error estimates for the mean and variance of the QoI with respect to the finite element, sparse grid and perturbation approximations. In section 7 a complexity and tolerance analysis is derived. Finally, in section 8 numerical examples are presented.

2. BACKGROUND

In this section we introduce the general notation and mathematical background that will be used in this paper. Let Ω be the set of outcomes from the complete probability space $(\Omega, \mathcal{F}, \mathbb{P})$, where \mathcal{F} is a sigma algebra of events and \mathbb{P} is a probability measure. Define $L_{\mathbb{P}}^q(\Omega)$, $q \in [1, \infty]$, as the following Banach spaces:

$$L_{\mathbb{P}}^q(\Omega) := \{v \mid \int_{\Omega} |v(\omega)|^q d\mathbb{P}(\omega) < \infty\} \text{ and } L_{\mathbb{P}}^{\infty}(\Omega) := \{v \mid \text{ess sup}_{\omega \in \Omega} |v(\omega)| < \infty\},$$

where $v : \Omega \rightarrow \mathbb{R}$ is a measurable random variable.

Let $\mathbf{Y} := [Y_1, \dots, Y_N]$ be a N valued random vector measurable in $(\Omega, \mathcal{F}, \mathbb{P})$ and without loss of generality denote $\Gamma_n := [-1, 1]$ as the image of Y_n for $n = 1, \dots, N$. Assume that \mathbf{Y} takes values on $\Gamma := \Gamma_1 \times \dots \times \Gamma_N \subset \mathbb{R}^N$ and let $\mathcal{B}(\Gamma)$ be the Borel σ - algebra. Define the induced measure $\mu_{\mathbf{Y}}$ on $(\Gamma, \mathcal{B}(\Gamma))$ as $\mu_{\mathbf{Y}} := \mathbb{P}(\mathbf{Y}^{-1}(A))$ for all $A \in \mathcal{B}(\Gamma)$. Assuming that the induced measure is absolutely continuous with respect to the Lebesgue measure defined on Γ , then there exists a density function $\rho(\mathbf{y}) : \Gamma \rightarrow [0, +\infty)$ such that for any event $A \in \mathcal{B}(\Gamma)$

$$\mathbb{P}(\mathbf{Y} \in A) := \mathbb{P}(\mathbf{Y}^{-1}(A)) = \int_A \rho(\mathbf{y}) d\mathbf{y}.$$

Now, for any measurable function $\mathbf{Y} \in L_P^1(\Gamma)$ define the expected value as

$$\mathbb{E}[\mathbf{Y}] = \int_{\Gamma} \mathbf{y} \rho(\mathbf{y}) d\mathbf{y}.$$

Define also the following Banach spaces:

$$L_\rho^q(\Gamma) := \left\{ v \mid \int_\Omega |v(\mathbf{y})|^q \rho(\mathbf{y}) d\mathbf{y} < \infty \right\} \text{ and}$$

$$L_\rho^\infty(\Gamma) := \left\{ v \mid \operatorname{ess\,sup}_{\mathbf{y} \in \Gamma} |v(\mathbf{y})| < \infty \right\}.$$

We discuss in the next section an approach of approximating a given function $\tilde{f} \in L_\rho^q(\Gamma)$, which is sufficiently smooth, by multivariate polynomials and sparse grid interpolation.

2.1. Sparse Grids. Our goal is to find a compact and accurate approximation of a multivariate function $\tilde{f} : \Gamma \rightarrow \mathbb{R}$ with sufficient regularity. It is assumed that $\tilde{f} \in C^0(\Gamma; V)$ where

$$C^0(\Gamma; V) := \{ v : \Gamma \rightarrow V \text{ is continuous on } \Gamma \text{ and } \max_{\mathbf{y} \in \Gamma} \|v(\mathbf{y})\|_V < \infty \}$$

and V is a Banach space. Consider the univariate Lagrange interpolant along the n^{th} dimension of Γ

$$\mathcal{I}_n^{m(i)} : C^0(\Gamma_n) \rightarrow \mathcal{P}_{m(i)-1}(\Gamma_n),$$

where $i \geq 1$ denotes the level of approximation and $m(i)$ the number of collocation knots used to build the interpolation at level i such that $m(0) = 0$, $m(1) = 1$ and $m(i) < m(i+1)$ for $i \geq 1$. Furthermore let $\mathcal{I}_n^{m(0)} = 0$. The space $\mathcal{P}_{m(i)-1}(\Gamma_n)$ is the set of polynomials of degree at most $m(i) - 1$.

We can construct an interpolant by taking tensor products of $\mathcal{I}_n^{m(i)}$ along each dimension for $n = 1, \dots, N$. However, the number of collocation knots explodes exponentially with respect to the number of dimensions, thus limiting feasibility to small dimensions. Alternately, consider the difference operator along the n^{th} dimension

$$\Delta_n^{m(i)} := \mathcal{I}_n^{m(i)} - \mathcal{I}_n^{m(i-1)}.$$

The sparse grid approximation of $\tilde{f} \in C^0(\Gamma)$ is defined as

$$(1) \quad \mathcal{S}_w^{m,g}[\tilde{f}] = \sum_{\mathbf{i} \in \mathbb{N}_+^N : g(\mathbf{i}) \leq w} \bigotimes_{n=1}^N \Delta_n^{m(i_n)}(\tilde{f})$$

where $w \geq 0$, $w \in \mathbb{N}_+$ ($\mathbb{N}_+ := \mathbb{N} \cup \{0\}$), is the approximation level, $\mathbf{i} = (i_1, \dots, i_N) \in \mathbb{N}_+^N$, and $g : \mathbb{N}_+^N \rightarrow \mathbb{N}$ is strictly increasing in each argument. The sparse grid can also be re-written as

$$(2) \quad \mathcal{S}_w^{m,g}[\tilde{f}] = \sum_{\mathbf{i} \in \mathbb{N}_+^N : g(\mathbf{i}) \leq w} c(\mathbf{i}) \bigotimes_{n=1}^N \mathcal{I}_n^{m(i_n)}(\tilde{f}), \quad \text{with } c(\mathbf{i}) = \sum_{\substack{\mathbf{j} \in \{0,1\}^N : \\ g(\mathbf{i}+\mathbf{j}) \leq w}} (-1)^{|\mathbf{j}|}.$$

From the previous expression, we see that the sparse grid approximation is obtained as a linear combination of full tensor product interpolations. However, the constraint $g(\mathbf{i}) \leq w$ in (2) restricts the growth of tensor grids of high degree.

Let $\mathbf{m}(\mathbf{i}) = (m(i_1), \dots, m(i_N))$ and consider the ordered polynomial polynomial set

$$\Lambda^{m,g}(w) = \{ \mathbf{p} \in \mathbb{N}^N, \ g(\mathbf{m}^{-1}(\mathbf{p} + \mathbf{1})) \leq w \}.$$

Let $\mathbb{P}_{\Lambda^{m,g}(w)}(\Gamma)$ be the associated multivariate polynomial space

$$\mathbb{P}_{\Lambda^{m,g}(w)}(\Gamma) = \text{span} \left\{ \prod_{n=1}^N y_n^{p_n}, \text{ with } \mathbf{p} \in \Lambda^{m,g}(w) \right\}.$$

It can shown that $\mathcal{S}_w^{m,g}[\tilde{f}] \in \mathbb{P}_{\Lambda^{m,g}(w)}(\Gamma)$ (see e.g. [2]). Now, one of the most typical choices for m and g is given by the Smolyak (SM) formulas (see [20, 3, 2])

$$m(i) = \begin{cases} 1, & \text{for } i = 1 \\ 2^{i-1} + 1, & \text{for } i > 1 \end{cases} \quad \text{and} \quad g(\mathbf{i}) = \sum_{n=1}^N (i_n - 1).$$

This choice of m , combined with the choice of Clenshaw-Curtis (CC) interpolation points (extrema of Chebyshev polynomials) leads to nested sequences of one dimensional interpolation formulas and a sparse grid with a highly reduced number of points compared to the corresponding tensor grid (see [2]). Other choices are given by Total Degree (TD) and Hyperbolic Cross (HC).

It can also be shown that the TD, SM and HC anisotropic sparse approximation formulas can be readily constructed with improved convergence rates (see [17]). Moreover, in [6], the authors show convergence of anisotropic sparse grid approximations with infinite dimensions ($N \rightarrow \infty$).

In [16] the authors show the construction of quasi-optimal grids have been shown to have exponential convergence.

3. PROBLEM SETUP AND FORMULATION

Let $D(\omega) \subset \mathbb{R}^d$ be an open bounded domain with Lipschitz boundary $\partial D(\omega)$ that is shape dependent on the stochastic parameter $\omega \in \Omega$ and and a Lipschitz bounded open reference domain $U \subset \mathbb{R}^d$. Let the map $F(\omega) : U \rightarrow D(\omega)$ be a one-to-one for all $\omega \in \Omega$ and whose image coincides with $D(\omega)$. Furthermore denote $\partial F(\omega)$ as the Jacobian of $F(\omega)$ and suppose that F satisfies the following assumption.

Assumption 1. *Given a one-to-one map $F(\omega) : U \rightarrow D(\omega)$ there exist constants \mathbb{F}_{min} and \mathbb{F}_{max} such that*

$$0 < \mathbb{F}_{min} \leq \sigma_{min}(\partial F(\omega)) \text{ and } \sigma_{max}(\partial F(\omega)) \leq \mathbb{F}_{max} < \infty$$

almost everywhere in U and almost surely in Ω . We have denoted by $\sigma_{min}(\partial F(\omega))$ (and $\sigma_{max}(\partial F(\omega))$) the minimum (respectively maximum) singular value of the Jacobian $\partial F(\omega)$. In Figure 1 a cartoon example of the deformation of the reference domain U is shown.

Lemma 1. *Under Assumptions 1 it is immediate to prove the following results:*

- i) $L^2(D(\omega))$ and $L^2(U)$ are isomorphic almost surely.
- ii) $H^1(D(\omega))$ and $H^1(U)$ are isomorphic almost surely.

Proof. see [5]. □

Now, consider the following boundary value problem: Given $f(\cdot, \omega), a(\cdot, \omega) : D(\omega) \rightarrow \mathbb{R}^d$ and $g(\cdot, \omega) : \partial D(\omega) \rightarrow \mathbb{R}^d$ find $u(\cdot, \omega) : D(\omega) \rightarrow \mathbb{R}^d$ such that almost surely

$$(3) \quad \begin{aligned} -\nabla \cdot (a(x, \omega) \nabla u(x, \omega)) &= f(x, \omega), \quad x \in D(\omega) \\ u &= g \quad \text{on } \partial D(\omega). \end{aligned}$$

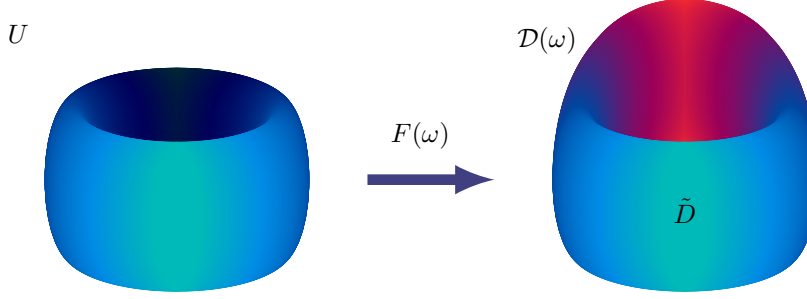


FIGURE 1. Cartoon example of stochastic domain realization from a reference domain. The front of the torus, shown by the area \tilde{D} is not stochastic and thus not deformed. The back of the torus is deformed from the reference domain U . This figure is modified from the TikZ tex code from *Smooth map of manifolds and smooth spaces* by Andrew Stacey [21].

We now make the following assumption:

Assumption 2. *There exist constants a_{min} and a_{max} such that*

$$0 < a_{min} \leq a(x, \omega) \leq a_{max} < \infty \text{ for a.e. } x \in D(\omega), \text{ and a.s. } \omega \in \Omega.$$

where

$$a_{min} := \operatorname{ess\,inf}_{x \in D(\omega), \omega \in \Omega} a(x, \omega) \text{ and } a_{max} := \operatorname{ess\,sup}_{x \in D(\omega), \omega \in \Omega} a(x, \omega).$$

Since U is bounded and Lipschitz there exists a bounded linear operator $T : H^{1/2}(\partial U) \rightarrow H^1(U)$ such that for all $\tilde{g} \in H^{1/2}(\partial U)$ we have that $\tilde{\mathbf{w}} := T\tilde{g} \in H^1(U)$ satisfies $\tilde{\mathbf{w}}|_U = \tilde{g}$ almost surely. By applying a change of variables the weak form of (3) can be reformulated on the reference domain U (see [5] for details) as:

Problem 1. *Given that $(f \circ F)(\cdot, \omega) \in L^2(U)$ find $\hat{u}(\cdot, \omega) \in H_0^1(U)$ s.t.*

$$(4) \quad B(\omega; \hat{u}, v) = \tilde{l}(\omega; v), \quad \forall v \in H_0^1(U)$$

almost surely, where $\tilde{l}(\omega; v) := \int_U (f \circ F)(\cdot, \omega) |\partial F(\cdot, \omega)| v - L(\hat{\mathbf{w}}(\cdot, \omega), v)$, $\hat{g} := g \circ F$, $\hat{\mathbf{w}} := T(\hat{g})$, for any $w, s \in H_0^1(U)$

$$B(\omega; s, w) := \int_U (a \circ F(\cdot, \omega) \nabla s^T C^{-1}(\cdot, \omega) \nabla w |\partial F(\cdot, \omega)|),$$

$$L(\hat{\mathbf{w}}(\cdot, \omega), v) := \int_U (a \circ F(\cdot, \omega) (\nabla(\hat{\mathbf{w}}(\cdot, \omega))^T C^{-1}(\cdot, \omega) |\partial F(\cdot, \omega)| \nabla v),$$

$C(\cdot, \omega) := \partial F(\omega)^T \partial F(\omega)$, and $\hat{\mathbf{w}}(\cdot, \omega)|_{\partial U} = \hat{g}(\cdot, \omega)$. This homogeneous boundary value problem can be remapped to $D(\omega)$ as $\tilde{u}(\cdot, \omega) := (\hat{u} \circ F^{-1})(\cdot, \omega)$, thus we can rewrite $\hat{u}(\cdot, \omega) = (\tilde{u} \circ F)(\cdot, \omega)$.

The solution $u(\cdot, \omega) \in H^1(D(\omega))$ for the Dirichlet boundary value problem is obtained as $u(\cdot, \omega) = \tilde{u}(\cdot, \omega) + (\hat{\mathbf{w}} \circ F^{-1})(\cdot, \omega)$.

3.1. Quantity of interest and the adjoint problem. For many practical problems the QoI is not necessarily the solution of the elliptic PDE, but instead a bounded linear functional $Q : H_0^1(U) \rightarrow \mathbb{R}$ of the solution. This could be for example the average of the solution on a specific region of the domain. Let us consider the QoI of the form

$$(5) \quad Q(u) := \int_{\tilde{D}} q(x)u(x, \omega) \, dx$$

with $q \in L^2(\tilde{D})$ over the region $\tilde{D} \subset D(\omega)$ for any $\omega \in \Omega$. It is assumed that there $\exists \delta > 0$ such that $\text{dist}(\tilde{D}, \partial D(\omega)) > \delta$ for all $\omega \in \Omega$ and $F|_{\tilde{D}} = I$ on \tilde{D} . In layman's terms the region \tilde{D} has no deformations and it is contained inside D . This, for example, could be a small patch inside D that is known not to be deformed.

Remark 1. *The restriction $F|_{\tilde{D}} = I$ on \tilde{D} is not hard. This is done to simplify the numerical simulations in Section 8. The perturbation approach in Section 4 and the analyticity analysis in Section 5 are still valid even if this restriction is relaxed.*

In the next section, the perturbation approximation is derived for $Q(u)$ and not directly from the solution u . It is thus necessary to introduce the influence function $\varphi : H_0^1(U) \rightarrow \mathbb{R}$, that can be easily computed by the following adjoint problem:

Problem 2. *Find $\varphi \in H_0^1(U)$ such that for all $v \in H_0^1(U)$*

$$(6) \quad B(\omega; v, \varphi) = Q(v)$$

a.s. in Ω . After computing the influence function φ , the QoI can be computed as $Q(u) = B(u, \varphi)$.

Remark 2. *We can pick a particular operator T such that $\hat{\mathbf{w}} = T(\hat{g})$ and vanishes in the region defined by \tilde{D} . Thus we have that $Q(\hat{\mathbf{w}}) = 0$ and $Q(u) = Q(\tilde{u} + \hat{\mathbf{w}}) = Q(\tilde{u})$.*

3.2. Domain parameterization and semi-discrete approximation. To simplify the analysis of the elliptic PDE with a random domain from equation (3) we remapped the solution onto a fix deterministic reference domain. This approach has also been applied in [7, 5]. We now restrict our attention to a particular class of domain deformation.

Assumption 3. *The map $F(\omega) : U \rightarrow D(\omega)$ has the form*

$$F(x, \omega) := x + e(x, \omega)\hat{v}(x)$$

a.s. in Ω , with $\hat{v} : U \rightarrow \mathbb{R}^d$, $\hat{v} := [\hat{v}_1, \dots, \hat{v}_d]^T$, $\hat{v}_i \in C^1(U)$ for $i = 1, \dots, d$, and $e(\cdot, \omega) : U \rightarrow D(\omega)$. Assume that the map $F(\omega) : U \rightarrow D(\omega)$ is one-to-one almost surely.

The magnitude of the stochastic domain perturbation is assumed to be parameterized as

$$e(x, \omega) := \sum_{n=1}^N \sqrt{\mu_n} b_n(x) Y_n(\omega).$$

Recall that for $n = 1, \dots, N$ let $\Gamma_n \equiv Y_n(\Omega)$, $\Gamma_n \equiv [-1, 1]$ and $\Gamma := \prod_{n=1}^{N_s} \Gamma_{N_s}$. Denote $\rho(\mathbf{y}_s) : \Gamma_s \rightarrow \mathbb{R}_+$ as the joint probability density of \mathbf{Y} . Now, the stochastic domain perturbation is split as

$$e(x, \omega) \rightarrow e_s(x, \omega) + e_f(x, \omega),$$

where we denote $e_s(x, \omega)$ as the large deviations and $e_f(x, \omega)$ as the small deviations modes with the following parameterization:

$$e_s(x, \omega) := \sum_{n=1}^{N_s} \sqrt{\mu_{s,n}} b_{s,n}(x) Y_n(\omega) \quad \text{and} \quad e_f(x, \omega) := \sum_{n=1}^{N_f} \sqrt{\mu_{f,n}} b_{f,n}(x) Y_{n+N_s}(\omega),$$

where $N_s + N_f = N$. Furthermore, for $n = 1, \dots, N_s$ let $\mu_{s,n} := \mu_n$, $b_{s,n}(x) := b_n(x)$, and for $n = 1, \dots, N_f$ let $\mu_{f,n} := \mu_{n+N_s}$ and $b_{f,n}(x) := b_{n+N_s}(x)$.

Denote $\mathbf{Y}_s := [Y_1, \dots, Y_{N_s}]$, $\Gamma_s := \prod_{n=1}^{N_s} \Gamma_n$, and $\rho(\mathbf{y}_s) : \Gamma_s \rightarrow \mathbb{R}_+$ as the joint probability density of \mathbf{Y}_s . Similarly denote $\mathbf{Y}_f := [Y_{N_s+1}, \dots, Y_N]$, $\Gamma_f := \prod_{n=N_s+1}^N \Gamma_n$, and $\rho(\mathbf{y}_f) : \Gamma_f \rightarrow \mathbb{R}_+$ as the joint probability density of \mathbf{Y}_f .

Assumption 4.

- (1) $b_1, \dots, b_N \in W^{2,\infty}(U)$
- (2) $\|b_n\|_{L^\infty(U)} = 1$ for $n = 1, 2, \dots, N$
- (3) μ_n are monotonically decreasing for $n = 1, 2, \dots, N$.
- (4) $\mathbb{E}[Y_n Y_m] = \delta[n - m]$, where $m, n = 1, \dots, N$.

Now, from the stochastic model the Jacobian ∂F is written as

$$(7) \quad \partial F(x, \omega) = I + \sum_{l=1}^N B_l(x) \sqrt{\mu_l} Y_l(\omega)$$

where i) for $l = 1, \dots, N_s$, $\sqrt{\mu_l} := \sqrt{\mu_{s,l}}$, $B_l := B_{s,l}$ and

$$B_{s,l}(x) := b_{s,l}(x) \partial \hat{v}(x) + \hat{v}(x) \nabla b_{s,l}(x)^T$$

where ∂v is the Jacobian of $v(x)$; ii) for $l = 1, \dots, N_f$ $\sqrt{\mu_{l+N_s}} := \sqrt{\mu_{f,l}}$, $B_{l+N_s} := B_{f,l}$ and similar definition for $B_{f,l}$.

Assumption 5.

- (1) $a \circ F$ and \hat{g} are only a function of $x \in U$ and independent of $\omega \in \Omega$.
- (2) There exists $0 < \tilde{\delta} < 1$ such that $\sum_{l=1}^N \|B_l(x)\|_2 \sqrt{\mu_l} \leq 1 - \tilde{\delta}$, for all $x \in U$.
- (3) Assume that $f : \mathbb{R}^d \rightarrow \mathbb{R}$ can be analytically extended in \mathbb{C}^d .

Let $H_h(U) \subset H_0^1(U)$ be the standard finite element space of dimension N_h , which contains continuous piecewise polynomials defined on regular triangulations \mathcal{T}_h that have a maximum mesh spacing parameter $h > 0$. Let $\hat{u}_h : \Gamma_s \rightarrow H_h(U)$ be the semi-discrete approximation that is obtained by projecting the solution of (4) onto the subspace $H_h(U)$, for each $\mathbf{y}_s \in \Gamma_s$, i.e.,

$$(8) \quad \int_U [\nabla \hat{u}_h(\cdot, \mathbf{y}_s)]^T G(\mathbf{y}_s) \nabla v_h \, dx = \int_U (f \circ F)(\cdot, \mathbf{y}_s) v_h |\partial F|(\mathbf{y}_s) \, dx - L(\hat{\mathbf{w}}, v_h)$$

for all $v_h \in H_h(U)$ and for a.s. $\mathbf{y}_s \in \Gamma$. Note that $G(\mathbf{y}_s) := (a \circ F(\mathbf{y}_s)) \det(\partial F(\mathbf{y}_s)) \partial F(\mathbf{y}_s)^{-1} \partial F(\mathbf{y}_s)^{-T}$ and $Q_h(\mathbf{y}_s) := Q(\hat{u}_h \circ F) = Q(\hat{u}_h(\mathbf{y}_s))$.

4. PERTURBATION

In this section we present a perturbation approach to approximate $Q(\mathbf{y})$ with respect to the domain perturbation. In Section 4.1, the perturbation approach is applied with respect to the tail field $e_f(\cdot, \omega)$. A stochastic collocation approach is then used to approximate the contribution with respect to $e_s(\cdot, \omega)$.

Whenever the perturbation of $Q(\mathbf{y}) := Q((\tilde{u} \circ F)(\cdot, \mathbf{y}))$ is small with respect to the parameters $\mathbf{y} \in W$, for a suitable linear vector space W of perturbations, a linear approximation is sufficient for an accurate estimate. To this end we introduce the following definition.

Definition 1. Let ψ be a regular function of the parameters $\mathbf{y} \in W$, the Gateaux derivative evaluated at \mathbf{y} on the space of perturbations W is defined as

$$\langle D_{\mathbf{y}}\psi(\mathbf{y}), \delta\mathbf{y} \rangle = \lim_{s \rightarrow 0^+} \frac{\psi(\mathbf{y} + s\delta\mathbf{y}) - \psi(\mathbf{y})}{s}, \forall \delta\mathbf{y} \in W.$$

Similarly, the second order derivative $D_{\mathbf{y}}^2$ as a bilinear form on W is defined as

$$D_{\mathbf{y}}^2\psi(\mathbf{y})(\delta\mathbf{y}_1, \delta\mathbf{y}_2) = \lim_{s \rightarrow 0^+} \langle \frac{D_{\mathbf{y}}\psi(\mathbf{y} + s\delta\mathbf{y}_2) - D_{\mathbf{y}}\psi(\mathbf{y})}{s}, \delta\mathbf{y}_1 \rangle, \forall \delta\mathbf{y}_2, \delta\mathbf{y}_1 \in W.$$

Suppose that Q is a regular function with respect to the parameters \mathbf{y} , then for all $\mathbf{y} = \mathbf{y}_0 + \delta\mathbf{y} \in W$ the following expansion holds:

$$(9) \quad Q(\mathbf{y}) = Q(\mathbf{y}_0) + \langle D_{\mathbf{y}}Q(\mathbf{y}_0), \delta\mathbf{y} \rangle + \frac{1}{2}D_{\mathbf{y}}^2Q(\mathbf{y} + \theta\delta\mathbf{y})(\delta\mathbf{y}, \delta\mathbf{y})$$

for some $\theta \in (0, 1)$. Thus we have a procedure to approximate the QoI $Q(\mathbf{y})$ with respect to the first order term and bound the error with the second order term. To explicitly formulate the first and second order terms we make the following assumption:

Assumption 6. For all $v, w \in H_0^1(U)$, let $\mathcal{G}(\mathbf{y}; v, w) := \nabla v^T G(\mathbf{y}) \nabla w$, where $G(\mathbf{y}) := (a \circ F)(\cdot, \mathbf{y}) \partial F^{-1}(\mathbf{y}) \partial F^{-T}(\mathbf{y}) |\partial F(\mathbf{y})|$, we have that for all $\mathbf{y} \in W$

- (i) $\nabla_{\mathbf{y}}\mathcal{G}(\mathbf{y}) \in [L^1(U)]^N$
- (ii) For $i = 1, \dots, N$ there exists $\mathcal{C}_{\mathcal{G}}(\mathbf{y}) > 0$ s.t.

$$\int_U \partial y_i \mathcal{G}(\mathbf{y}; v, w) \leq \mathcal{C}_{\mathcal{G}}(\mathbf{y}) \|v\|_{H_0^1(U)} \|w\|_{H_0^1(U)}.$$

- (iii) $\mathcal{C}_{\mathcal{G}}(\mathbf{y})$ is uniformly bounded on W .

Furthermore, for all $\mathbf{y} \in \mathcal{A}_{\mathbf{y}}$ we have that $\nabla_{\mathbf{y}}(f \circ F)(\mathbf{y}), \nabla_{\mathbf{y}}\hat{\mathbf{w}}(\mathbf{y}) \in [L^1(U)]^N$

Remark 3. Although we have that (i) - (iii) are assumptions for now, under Assumptions 1 - 4 and Lemma 8 in Section 6 it can be shown that Assumption 6(i) - (iii) are true for all $\mathbf{y} \in \Gamma$.

Definition 2. For all $v, w \in H_0^1(U)$, and $\mathbf{y} \in W$ let

$$\langle D_{\mathbf{y}}B(\mathbf{y}; v, w), \delta\mathbf{y} \rangle := \lim_{s \rightarrow 0^+} \frac{1}{s} [B(\mathbf{y} + s\delta\mathbf{y}; v, w) - B(\mathbf{y}; v, w)] \quad \forall \delta\mathbf{y} \in W.$$

Remark 4. Under Assumption 6 for $v, w \in H_0^1(U)$ we have that for all $\mathbf{y} \in W$

$$\langle D_{\mathbf{y}}B(\mathbf{y}; v, w), \delta\mathbf{y} \rangle = \int_U \nabla_{\mathbf{y}}\mathcal{G}(\mathbf{y}; v, w) \cdot \delta\mathbf{y} = \sum_{n=1}^N \int_U (\nabla v^T \partial y_n G(\mathbf{y}) \nabla w) \delta y_n$$

Furthermore, under Assumption 6 we have that

$$\langle D_{\mathbf{y}}(f \circ F)(\cdot, \mathbf{y}), \delta \mathbf{y} \rangle = \int_U \nabla_{\mathbf{y}}(f \circ F)(\cdot, \mathbf{y}) \cdot \delta \mathbf{y}.$$

We can introduce as well the derivative for any function $(v \circ F)(\cdot, \mathbf{y}) \in L^2(U)$ with respect to \mathbf{y} : For all $\mathbf{y} \in W$ we have that

$$D_{\mathbf{y}}(v \circ F)(\cdot, \mathbf{y})(\delta \mathbf{y}) := \lim_{s \rightarrow 0^+} \frac{1}{s} [(v \circ F)(\cdot, \mathbf{y} + s\delta \mathbf{y}) - (v \circ F)(\cdot, \mathbf{y})].$$

Finally, we assume that Assumptions 1 & 2 and Problems 1 & 2 are valid for the \mathbb{R}^N valued vector $\mathbf{y} \in W$. This is only to show that the perturbation approach is valid for the general set of perturbations in W . We then use this result in Section 4.1 for the allowable perturbations $\mathbf{y} \in \Gamma$.

Lemma 2. *Suppose that Assumptions 1, 2 and 6 are satisfied then for any $\mathbf{y}, \delta \mathbf{y} \in W$ and for all $v \in H_0^1(U)$ we have that*

$$\begin{aligned} B(\mathbf{y}; D_{\mathbf{y}}(\tilde{u} \circ F)(\cdot, \mathbf{y})(\delta \mathbf{y}), v) &= \sum_{n=1}^N \delta y_n \left(\int_U -(\nabla(\tilde{u} \circ F)(\cdot, \mathbf{y}))^T \partial_{y_n} G(\mathbf{y}) \nabla v \right. \\ &\quad + \partial_{y_n}(f \circ F)(\cdot, \mathbf{y}) |\partial F(\mathbf{y})| v + (f \circ F)(\cdot, \mathbf{y}) \partial_{y_n} |\partial F(\mathbf{y})| v \\ &\quad \left. - (\nabla \mathbf{w}(\mathbf{y}))^T \partial_{y_n} G(\mathbf{y}) \nabla v - (\partial_{y_n} \nabla \mathbf{w}(\mathbf{y}))^T G(\mathbf{y}) \nabla v \right). \end{aligned}$$

Proof.

$$\begin{aligned} B(\mathbf{y}; D_{\mathbf{y}}(\tilde{u} \circ F)(\cdot, \mathbf{y})(\delta \mathbf{y}), v) &= \lim_{s \rightarrow 0^+} \frac{1}{s} \int_U (\nabla(\tilde{u} \circ F)(\cdot, \mathbf{y} + s\delta \mathbf{y}))^T \\ &\quad - \nabla(\tilde{u} \circ F)(\cdot, \mathbf{y})^T G(\mathbf{y}) \nabla v \\ &= \lim_{s \rightarrow 0^+} \frac{1}{s} \int_U \nabla(\tilde{u} \circ F)(\cdot, \mathbf{y} + s\delta \mathbf{y})^T G(\mathbf{y}) \nabla v \\ &\quad - \nabla(\tilde{u} \circ F)(\cdot, \mathbf{y} + s\delta \mathbf{y})^T G(\mathbf{y} + s\delta \mathbf{y}) \nabla v \\ &\quad + \lim_{s \rightarrow 0^+} \frac{1}{s} \int_U \nabla(\tilde{u} \circ F)(\cdot, \mathbf{y} + s\delta \mathbf{y})^T G(\mathbf{y} + s\delta \mathbf{y}) \nabla v - \nabla(\tilde{u} \circ F)(\cdot, \mathbf{y})^T G(\mathbf{y}) \nabla v \\ &= - \sum_{i=1}^N \int_U (\nabla(\tilde{u} \circ F)(\cdot, \mathbf{y}))^T \partial_{y_i} G(\mathbf{y}) \delta y_i \nabla v \\ &\quad + \lim_{s \rightarrow 0^+} \frac{1}{s} \left(\tilde{l}(\mathbf{y} + s\delta \mathbf{y}; v) - \tilde{l}(\mathbf{y}; v) \right) \end{aligned}$$

then

$$\begin{aligned} B(\mathbf{y}; D_{\mathbf{y}}(\tilde{u} \circ F)(\cdot, \mathbf{y})(\delta \mathbf{y}), v) &= \sum_{n=1}^N \int_U -\nabla(\tilde{u} \circ F)(\cdot, \mathbf{y})^T \partial_{y_n} G(\mathbf{y}) \delta y_n \nabla v \\ &\quad + \int_U \partial_{y_n}(f \circ F)(\cdot, \mathbf{y}) \delta y_n |\partial F(\mathbf{y})| v + \int_U (f \circ F)(\cdot, \mathbf{y}) \partial_{y_n} |\partial F(\mathbf{y})| \delta y_n v \\ &\quad - \lim_{s \rightarrow 0^+} \frac{1}{s} \int_U (\nabla \hat{\mathbf{w}}(\mathbf{y} + s\delta \mathbf{y}))^T G(\mathbf{y} + s\delta \mathbf{y}) \nabla v - (\nabla \hat{\mathbf{w}}(\mathbf{y}))^T G(\mathbf{y}) \nabla v \end{aligned}$$

The result follows. \square

Lemma 3. *Suppose that Assumptions 1, 2 and 6 are satisfied then for any $\mathbf{y}, \delta\mathbf{y} \in W$ and for all $v \in H_0^1(U)$ we have that*

$$B(\mathbf{y}; v, D_{\mathbf{y}}\varphi(\mathbf{y})(\delta\mathbf{y})) = \sum_{i=1}^N \int_U -(\nabla v)^T \partial_{y_i} G(\mathbf{y}) \delta y_i \nabla \varphi(\mathbf{y}).$$

Proof. We follow the same procedure as in Lemma 2. □

Remark 5. *A consequence of Lemma 2 and Lemma 3 is that if for $n = 1, \dots, N_f$ the terms $\|\partial_{y_n} G(\mathbf{y})\|_2$, $|\partial_{y_n} \det(\partial F(\mathbf{y}))|$, $\|\partial_{y_n} (f \circ F)(\cdot, \mathbf{y})\|_{L^2(U)}$ and $\|\partial_{y_n} \mathbf{w}(\cdot, \mathbf{y})\|_{H_0^1(U)}$ are uniformly bounded for all $\mathbf{y} \in W$ then $D_{\mathbf{y}}(\tilde{u} \circ F)(\cdot, \mathbf{y})(\delta\mathbf{y})$ and $D_{\mathbf{y}}\varphi(\mathbf{y})(\delta\mathbf{y})$ belong in $H_0^1(U)$ for any $\mathbf{y} \in W$ and $\delta\mathbf{y} \in W$.*

Lemma 4. *Under the same assumption as Lemma 3 we have that*

$$\begin{aligned} \lim_{s \rightarrow 0^+} \frac{Q(\mathbf{y} + s\delta\mathbf{y}) - Q(\mathbf{y})}{s} &= \sum_{i=n}^N \delta y_i \int_U \left(-(\nabla(\tilde{u} \circ F)(\cdot, \mathbf{y}))^T \partial_{y_n} G(\mathbf{y}) \nabla \varphi(\mathbf{y}) \right. \\ (10) \quad &+ \partial_{y_n} (f \circ F)(\cdot, \mathbf{y}) |\partial F(\mathbf{y})| \varphi(\mathbf{y}) - (\nabla \partial_{y_n} \mathbf{w}(\mathbf{y}))^T G(\mathbf{y}) \nabla \varphi(\mathbf{y}) \\ &\left. - (\nabla \mathbf{w}(\mathbf{y}))^T \partial_{y_n} G(\mathbf{y}) \nabla \varphi(\mathbf{y}) + (f \circ F)(\cdot, \mathbf{y}) \partial_{y_n} |\partial F(\mathbf{y})| \varphi(\mathbf{y}) \right). \end{aligned}$$

where the influence function $\varphi(\mathbf{y})$ satisfies equation (6).

Proof.

$$\begin{aligned} \lim_{s \rightarrow 0^+} \frac{Q(\mathbf{y} + s\delta\mathbf{y}) - Q(\mathbf{y})}{s} &= \lim_{s \rightarrow 0^+} \int_U \frac{1}{s} (\nabla(\tilde{u} \circ F)(\cdot, \mathbf{y} + s\delta\mathbf{y}))^T G(\mathbf{y} + s\delta\mathbf{y}) \nabla \varphi(\mathbf{y} + s\delta\mathbf{y}) \\ &\quad - (\nabla(\tilde{u} \circ F)(\cdot, \mathbf{y}))^T G(\mathbf{y}) \nabla \varphi(\mathbf{y}) \\ &= \sum_{n=1}^N \delta y_n \int_U (\nabla(\tilde{u} \circ F)(\cdot, \mathbf{y}))^T \partial_{y_n} G(\mathbf{y}) \nabla \varphi(\mathbf{y}) \\ &\quad + \int_U (\nabla D_{\mathbf{y}}(\tilde{u} \circ F)(\cdot, \mathbf{y}))^T (\delta\mathbf{y}) G(\mathbf{y}) \nabla \varphi(\mathbf{y}) \\ &\quad + (\nabla(\tilde{u} \circ F)(\cdot, \mathbf{y}))^T G(\mathbf{y}) \nabla D_{\mathbf{y}}\varphi(\mathbf{y})(\delta\mathbf{y}). \end{aligned}$$

From Lemma 2 with $v = \varphi(\mathbf{y})$ and Lemma 3 with $v = (\tilde{u} \circ F)(\cdot, \mathbf{y})$ we obtain the result. □

Lemma 5. *Suppose that Assumptions 1, 2 and 6 are satisfied then for any $\mathbf{y}, \delta\mathbf{y} \in W$ and for all $v \in H_0^1(U)$ we have that*

$$\begin{aligned}
D_{\mathbf{y}}^2 Q(\mathbf{y})(\delta\mathbf{y}, \delta\mathbf{y}) = & - \sum_{n,m=1}^N \delta y_n \delta y_m \left(\int_U (\nabla(\tilde{u} \circ F)(\cdot, \mathbf{y}))^T (\partial_{y_m} \partial_{y_n} G(\mathbf{y})) \nabla \varphi(\mathbf{y}) \right. \\
& + (\nabla \partial_{y_m} \partial_{y_n} \mathbf{w}(\mathbf{y}))^T G(\mathbf{y}) \nabla \varphi(\mathbf{y}) + (\nabla \partial_{y_n} \mathbf{w}(\mathbf{y}))^T \partial_{y_m} G(\mathbf{y}) \nabla \varphi(\mathbf{y}) \\
& + (\nabla \partial_{y_m} \mathbf{w}(\mathbf{y}))^T \partial_{y_n} G(\mathbf{y}) \nabla \varphi(\mathbf{y}) + (\nabla \mathbf{w}(\mathbf{y}))^T \partial_{y_m} \partial_{y_n} G(\mathbf{y}) \nabla \varphi(\mathbf{y}) \\
& - \partial_{y_m} \partial_{y_n} (f \circ F)(\cdot, \mathbf{y}) |\partial F(\mathbf{y})| \varphi(\mathbf{y}) - \partial_{y_n} (f \circ F)(\cdot, \mathbf{y}) \partial_{y_m} |\partial F(\mathbf{y})| \varphi(\mathbf{y}) \\
& \left. - \partial_{y_m} (f \circ F)(\cdot, \mathbf{y}) \partial_{y_n} |\partial F(\mathbf{y})| \varphi(\mathbf{y}) - (f \circ F)(\cdot, \mathbf{y}) \partial_{y_m} \partial_{y_n} |\partial F(\mathbf{y})| \varphi(\mathbf{y}) \right) \\
& - \sum_{n=1}^N \delta y_n \left(\int_U (\nabla D_{\mathbf{y}}(\tilde{u} \circ F)(\cdot, \mathbf{y}))^T (\delta\mathbf{y}) (\partial_{y_n} G(\mathbf{y})) \nabla \varphi(\mathbf{y}) \right. \\
& + (\nabla(\tilde{u} \circ F)(\cdot, \mathbf{y}))^T (\partial_{y_n} G(\mathbf{y})) \nabla D_{\mathbf{y}} \varphi(\mathbf{y})(\delta\mathbf{y}) + (\nabla \partial_{y_n} \mathbf{w}(\mathbf{y}))^T G(\mathbf{y}) \nabla D_{\mathbf{y}} \varphi(\mathbf{y})(\delta\mathbf{y}) \\
& + (\nabla \mathbf{w}(\mathbf{y}))^T \partial_{y_n} G(\mathbf{y}) \nabla D_{\mathbf{y}} \varphi(\mathbf{y})(\delta\mathbf{y}) - \partial_{y_n} (f \circ F)(\cdot, \mathbf{y}) |\partial F(\mathbf{y})| D_{\mathbf{y}} \varphi(\mathbf{y})(\delta\mathbf{y}) \\
& \left. - (f \circ F)(\cdot, \mathbf{y}) \partial_{y_n} |\partial F(\mathbf{y})| D_{\mathbf{y}} \varphi(\mathbf{y})(\delta\mathbf{y}) \right).
\end{aligned}$$

Proof. Taking the first variation of equation (10) we obtain the result. \square

4.1. Hybrid collocation-perturbation approach. We now consider a linear approximation of the QoI $Q(\mathbf{y})$ with respect to \mathbf{y} . For any $\mathbf{y} = \mathbf{y}_0 + \delta\mathbf{y}$, $\mathbf{y}_0 \in \mathbb{R}^N$, $\mathbf{y} \in \mathbb{R}^N$, the linear approximation has the form

$$Q^{linear}(\mathbf{y}) := Q(\mathbf{y}_0) + \langle D_{\mathbf{y}} Q(\mathbf{y}_0), \delta\mathbf{y} \rangle$$

where $\delta\mathbf{y} = \mathbf{y} - \mathbf{y}_0 \in \mathbb{R}^N$. recall that $\Gamma = \Gamma_s \times \Gamma_f$. Assume that

- i) $\mathbf{y} := [\mathbf{y}_s, \mathbf{y}_f]$, $\delta\mathbf{y} := [\delta\mathbf{y}_s, \delta\mathbf{y}_f]$, and $\mathbf{y}_0 := [\mathbf{y}^s, \mathbf{y}_0^f]$.
- ii) \mathbf{y}^s takes values on Γ_s and $\delta\mathbf{y}_s := \mathbf{0} \in \Gamma_s$.
- iii) $\mathbf{y}_0^f := \mathbf{0} \in \Gamma_f$ and $\delta\mathbf{y}_f = \mathbf{y}_f$ takes values on Γ_f .

We can now construct a linear approximation of the QoI with respect to the allowable perturbation set Γ . Consider the following linear approximation of $Q(\mathbf{y}_s, \mathbf{y}_f)$

$$(11) \quad \hat{Q}(\mathbf{y}_s, \mathbf{y}_f) := Q(\mathbf{y}_s, \mathbf{y}_0^f) + \tilde{Q}(\mathbf{y}_s, \mathbf{y}_0^f, \delta\mathbf{y}_f),$$

and from Lemma 4 we have that

$$\tilde{Q}(\mathbf{y}_s, \mathbf{y}_0^f, \delta\mathbf{y}_f) := \langle D_{\mathbf{y}} Q(\mathbf{y}_s, \mathbf{y}_0^f), \delta\mathbf{y}_0^f \rangle = \sum_{n=1}^{N_f} \delta y_n^f \int_U \alpha_n(x, \mathbf{y}_s, \mathbf{y}_0^f) dx,$$

where

$$\begin{aligned}
\alpha_n(\cdot, \mathbf{y}_s, \mathbf{y}_0^f) := & -(\nabla(\tilde{u} \circ F)(\cdot, \mathbf{y}_s, \mathbf{y}_0^f))^T \partial_{y_n^f} G(\mathbf{y}_s, \mathbf{y}_0^f) \nabla \varphi(\mathbf{y}_s) \\
& + \partial_{y_n^f} (f \circ F)(\cdot, \mathbf{y}_s, \mathbf{y}_0^f) |\partial F(\mathbf{y}_s, \mathbf{y}_0^f)| \varphi(\mathbf{y}_s, \mathbf{y}_0^f) \\
& - (\nabla \partial_{y_n^f} \mathbf{w}(\mathbf{y}_s, \mathbf{y}_0^f))^T G(\mathbf{y}_s, \mathbf{y}_0^f) \nabla \varphi(\mathbf{y}_s, \mathbf{y}_0^f) \\
& - (\nabla \mathbf{w}(\mathbf{y}_s, \mathbf{y}_0^f))^T \partial_{y_n^f} G(\mathbf{y}_s, \mathbf{y}_0^f) \nabla \varphi(\mathbf{y}_s, \mathbf{y}_0^f) \\
& + (f \circ F)(\cdot, \mathbf{y}_s, \mathbf{y}_0^f) \partial_{y_n^f} |\partial F(\mathbf{y}_s, \mathbf{y}_0^f)| \varphi(\mathbf{y}_s, \mathbf{y}_0^f).
\end{aligned}$$

Remark 6. *It is not hard to see that $\langle D_{\mathbf{y}}Q(\mathbf{y}_s, \mathbf{y}_0^f), \delta \mathbf{y}_0^f \rangle$ can be rewritten as*

$$(12) \quad \langle D_{\mathbf{y}}Q(\mathbf{y}_s, \mathbf{y}_0^f), \delta \mathbf{y}_0^f \rangle = \sum_{n=1}^{N_f} \sqrt{\mu_{f,n}} \delta y_n^f \int_U \tilde{\alpha}_n(x, \mathbf{y}_s, \mathbf{y}_0^f) dx$$

where

$$\begin{aligned} \tilde{\alpha}_n(\cdot, \mathbf{y}_s, \mathbf{y}_0^f) := & -(\nabla(\tilde{u} \circ F)(\cdot, \mathbf{y}_s, \mathbf{y}_0^f))^T \partial_{\tilde{y}_n^f} G(\mathbf{y}_s, \mathbf{y}_0^f) \nabla \varphi(\mathbf{y}_s, \mathbf{y}_0^f) \\ & + \partial_{\tilde{y}_n^f} (f \circ F)(\cdot, \mathbf{y}_s, \mathbf{y}_0^f) |\partial F(\mathbf{y}_s, \mathbf{y}_0^f)| \varphi(\mathbf{y}_s, \mathbf{y}_0^f) \\ & - (\nabla \partial_{\tilde{y}_n^f} \mathbf{w}(\mathbf{y}_s, \mathbf{y}_0^f))^T G(\mathbf{y}_s, \mathbf{y}_0^f) \nabla \varphi(\mathbf{y}_s, \mathbf{y}_0^f) \\ & - (\nabla \mathbf{w}(\mathbf{y}_s, \mathbf{y}_0^f))^T \partial_{\tilde{y}_n^f} G(\mathbf{y}_s, \mathbf{y}_0^f) \nabla \varphi(\mathbf{y}_s, \mathbf{y}_0^f) \\ & + (f \circ F)(\cdot, \mathbf{y}_s, \mathbf{y}_0^f) \partial_{\tilde{y}_n^f} |\partial F(\mathbf{y}_s, \mathbf{y}_0^f)| \varphi(\mathbf{y}_s, \mathbf{y}_0^f) \end{aligned}$$

and $\tilde{y}_n^f := y_n^f \sqrt{\mu_{f,n}}$ for $n = 1, \dots, N_f$. This will allow an explicit dependence of the mean and variance error in terms of the coefficients $\mu_{f,n}$, $n = 1, \dots, N_f$, as show in in Section 6.

The mean of $\hat{Q}(\mathbf{y}_s, \mathbf{y}_f)$ can be obtained as

$$\mathbb{E}[\hat{Q}(\mathbf{y}_s, \mathbf{y}_f)] = \mathbb{E}[Q(\mathbf{y}_s, \mathbf{y}_0^f)] + \mathbb{E}[\tilde{Q}(\mathbf{y}_s, \mathbf{y}_0^f, \delta \mathbf{y}_f)].$$

From Fubini's theorem we have

$$(13) \quad \mathbb{E}[Q(\mathbf{y}_s, \mathbf{y}_0^f)] = \int_{\Gamma_s} Q(\mathbf{y}_s, \mathbf{0}) \rho_s(\mathbf{y}_s) d\mathbf{y}_s.$$

and from equation (12)

$$(14) \quad \mathbb{E}[\tilde{Q}(\mathbf{y}_s, \mathbf{y}_0^f, \delta \mathbf{y}_f)] = \sum_{n=1}^{N_f} \sqrt{\mu_{f,n}} \int_{\Gamma_s} \int_{[-1,1]} y_n^f \gamma_n(\mathbf{y}_s, \mathbf{0}) \rho(\mathbf{y}_s, y_n^f) d\mathbf{y}_s dy_n^f,$$

where $\gamma_n(\mathbf{y}_s, \mathbf{0}) := \int_U \tilde{\alpha}_n(x, \mathbf{y}_s, \mathbf{0}) dx$, $\rho(\mathbf{y}_s)$ is the marginal distribution of $\rho(\mathbf{y})$ with respect to the variables \mathbf{y}_s and similarly for $\rho(\mathbf{y}_s, y_n^f)$ ($n = 1, \dots, N_f$). The term $\mathbb{E}[\tilde{Q}(\mathbf{y}_s, \mathbf{y}_0^f, \delta \mathbf{y}_f)]$ is referred as the *mean correction*.

The variance of $\hat{Q}(\mathbf{y}_s, \mathbf{y}_f)$ can be computed as

$$\begin{aligned} \text{var}[\hat{Q}(\mathbf{y}_s, \mathbf{y}_f)] = & \mathbb{E}[\hat{Q}(\mathbf{y}_s, \mathbf{y}_f)^2] - \mathbb{E}[\hat{Q}(\mathbf{y}_s, \mathbf{y}_f)]^2 = \text{var}[Q(\mathbf{y}_s, \mathbf{y}_0^f)] \\ & + \underbrace{\mathbb{E}[\tilde{Q}(\mathbf{y}_s, \mathbf{y}_0^f, \delta \mathbf{y}_f)^2] + 2\mathbb{E}[Q(\mathbf{y}_s, \mathbf{y}_0^f)\tilde{Q}(\mathbf{y}_s, \mathbf{y}_0^f, \delta \mathbf{y}_f)]}_{(I)} \\ & - \underbrace{\mathbb{E}[\tilde{Q}(\mathbf{y}_s, \mathbf{y}_0^f, \delta \mathbf{y}_f)]^2 - 2\mathbb{E}[Q(\mathbf{y}_s, \mathbf{y}_0^f)]\mathbb{E}[\tilde{Q}(\mathbf{y}_s, \mathbf{y}_0^f, \delta \mathbf{y}_f)]}_{(I)}. \end{aligned}$$

The term (I) is referred as the *variance correction* of $\text{var}[Q(\mathbf{y}_s, \mathbf{y}_0^f)]$. From Fubini's theorem and equation (12) we have that

$$(15) \quad \begin{aligned} \mathbb{E}[\tilde{Q}(\mathbf{y}_s, \mathbf{y}_0^f, \delta \mathbf{y}_f)^2] = & \sum_{k=1}^{N_f} \sum_{n=1}^{N_f} \int_{\Gamma_L} \int_{[-1,1]} \int_{[-1,1]} \sqrt{\mu_{f,k}} \sqrt{\mu_{f,n}} y_k^f y_n^f \\ & \gamma_j(\mathbf{y}_s, \mathbf{y}_0^f) \gamma_n(\mathbf{y}_s, \mathbf{y}_0^f) \rho(\mathbf{y}_s, y_k^f, y_n^f) d\mathbf{y}_s dy_k^f dy_n^f, \end{aligned}$$

and $\mathbb{E}[Q(\mathbf{y}_s, \mathbf{y}_0^f) \tilde{Q}(\mathbf{y}_s, \mathbf{y}_0^f, \delta \mathbf{y}_f)]$ is equal to

$$(16) \quad \sum_{k=1}^{N_f} \int_{\Gamma_s} \int_{[-1,1]} Q(\mathbf{y}_s, \mathbf{0}) \gamma_k(\mathbf{y}_s, \mathbf{0}) y_k^f \rho(\mathbf{y}_s, y_k^f) d\mathbf{y}_s dy_k^f.$$

Note that the mean $\mathbb{E}[Q(\mathbf{y}_s, \mathbf{y}_0^f)]$ and variance $\text{var}[Q(\mathbf{y}_s, \mathbf{y}_0^f)]$ depend only on the large variation variables \mathbf{y}_s . If the region of analyticity of the QoI with respect to the stochastic variables \mathbf{y}_s is large, it is reasonable to approximate $Q(\mathbf{y}_s, \mathbf{y}_0^f)$ with a Smolyak sparse grid $\mathcal{S}_w^{m,g}[Q(\mathbf{y}_s, \mathbf{y}_0^f)]$. Thus in equations (13) - (16) $Q(\mathbf{y}_s, \mathbf{y}_0^f)$ are replaced with the sparse grid approximation $\mathcal{S}_w^{m,g}[Q(\mathbf{y}_s, \mathbf{y}_0^f)]$ and for $n = 1, \dots, N_f$ $\gamma_n(\mathbf{y}_s, \mathbf{0})$ is replaced with $\mathcal{S}_w^{m,g}\gamma_n(\mathbf{y}_s, \mathbf{0})$.

Remark 7. For the special case that $\rho(\mathbf{y}) = \rho(\mathbf{y}_s)\rho(\mathbf{y}_f)$, for all $\mathbf{y}_s \in \Gamma_s$ and $\mathbf{y}_f \in \Gamma_f$ (i.e. independence assumption of the joint probability distribution $\rho(\mathbf{y}_s, \mathbf{y}_f)$), the mean and variance corrections are simplified. Applying Fubini's theorem and from equation 13 the mean of $\hat{Q}(\mathbf{y}_s, \mathbf{y}_f)$ now becomes

$$\begin{aligned} \mathbb{E}[\hat{Q}(\mathbf{y}_s, \mathbf{y}_f)] &= \mathbb{E}[Q(\mathbf{y}_s, \mathbf{y}_0^f)] + \underbrace{\mathbb{E}[\tilde{Q}(\mathbf{y}_s, \mathbf{y}_0^f, \delta \mathbf{y}_f)]}_{=0} = \mathbb{E}[Q(\mathbf{y}_s, \mathbf{y}_0^f)] \\ &= \int_{\Gamma_s} Q(\mathbf{y}_s, \mathbf{0}) \rho_s(\mathbf{y}_s) d\mathbf{y}_s, \end{aligned}$$

i.e. there is no contribution from the small variations. Applying a similar argument we have that

$$\begin{aligned} \text{var}[\hat{Q}(\mathbf{y}_s, \mathbf{y}_f)] &= \mathbb{E}[\hat{Q}(\mathbf{y}_s, \mathbf{y}_f)^2] - \mathbb{E}[\hat{Q}(\mathbf{y}_s, \mathbf{y}_f)]^2 = \text{var}[Q(\mathbf{y}_s, \mathbf{y}_0^f)] \\ &\quad + \mathbb{E}[\tilde{Q}(\mathbf{y}_s, \mathbf{y}_0^f, \delta \mathbf{y}_f)^2] + \underbrace{2\mathbb{E}[Q(\mathbf{y}_s, \mathbf{y}_0^f) \tilde{Q}(\mathbf{y}_s, \mathbf{y}_0^f, \delta \mathbf{y}_f)]}_{=0} \\ &\quad - \underbrace{\mathbb{E}[\tilde{Q}(\mathbf{y}_s, \mathbf{y}_0^f, \delta \mathbf{y}_f)]^2}_{=0} - 2 \underbrace{\mathbb{E}[Q(\mathbf{y}_s, \mathbf{y}_0^f)] \mathbb{E}[\tilde{Q}(\mathbf{y}_s, \mathbf{y}_0^f, \delta \mathbf{y}_f)]}_{=0} \\ &= \text{var}[Q(\mathbf{y}_s, \mathbf{y}_0^f)] + \underbrace{\sum_{n=1}^{N_f} \mu_n^f \int_U \alpha_n(x, \mathbf{y}_s, \mathbf{y}_0^f) dx \int_U \alpha_n(y, \mathbf{y}_s, \mathbf{y}_0^f) dy}_{\text{Variance correction}}. \end{aligned}$$

Notice that for this case the variance correction consists of N_f terms, thus the computational cost will depend linearly with respect to N_f .

5. ANALYTIC CORRECTION

In this section we show that the mean and variance corrections are analytic in a well defined region in \mathbb{C}^{N_s} with respect to the variables \mathbf{y}_s . The size of the regions of analyticity will directly correlated with the convergence rate of a Smolyak sparse grid. To this end, let us establish the following definition: For any $0 < \beta < \tilde{\delta}$, for some constant $\tilde{\delta} > 0$, define the following region in \mathbb{C}^{N_s} ,

$$(17) \quad \Theta_{\beta, N_s} := \left\{ \mathbf{z} \in \mathbb{C}^{N_s}; \mathbf{z} = \mathbf{y} + \mathbf{w}, \mathbf{y} \in [-1, 1]^{N_s}, \sum_{l=1}^{N_s} \sup_{x \in U} \|B_l(x)\|_2 \sqrt{\mu_l} |w_l| \leq \beta \right\}.$$

Observe that the size of the region Θ_{β, N_s} is mostly controlled by the decay of the coefficients μ_l and the size of $\|B_l(x)\|_2$. Thus the smaller and faster the coefficient μ_l decays the larger the region Θ_{β, N_s} will be.

Furthermore, rewrite $\partial F(\cdot, \omega)$ as $\partial F(\mathbf{y}) = I + R(\mathbf{y})$, with $R(\mathbf{y}) := \sum_{l=1}^N \sqrt{\mu_l} B_l(x) y_l$. We now state the first analyticity theorem for the solution $(\tilde{u} \circ F)(\mathbf{y}_s)$ with respect to the random variables $\mathbf{y} \in \Gamma$.

Theorem 1. *Let $0 < \tilde{\delta} < 1$ then the solution $(\tilde{u} \circ F)(\cdot, \mathbf{y}) : \Gamma \rightarrow H_0^1(U)$ of Problem 1 can be extended holomorphically on $\Theta_{\beta, N}$ if*

$$\beta < \min \left\{ \tilde{\delta} \frac{\log(2 - \gamma)}{d + \log(2 - \gamma)}, \sqrt{1 + \tilde{\delta}^2/2} - 1 \right\}$$

where $\gamma := \frac{2\tilde{\delta}^2 + (2 - \tilde{\delta})^d}{\tilde{\delta}^d + (2 - \tilde{\delta})^d}$.

Proof. See Theorem 7 in [5]. □

Remark 8. *By following a similar argument, the influence function $\varphi(\mathbf{y})$ can be extended holomorphically in $\Theta_{\beta, N}$ if*

$$\beta < \min \left\{ \tilde{\delta} \frac{\log(2 - \gamma)}{d + \log(2 - \gamma)}, \sqrt{1 + \tilde{\delta}^2/2} - 1 \right\}$$

We are now ready to show that the linear approximation $\hat{Q}(\mathbf{y}_s, \mathbf{y}_f)$ can be analytically extended on Θ_{β, N_s} . Note that it is sufficient to show that $\int_U \tilde{\alpha}_n(\cdot, \mathbf{y}_s, \mathbf{0})$ can be analytically extended on Θ_{β, N_s} .

Theorem 2. *Let $0 < \tilde{\delta} < 1$, if $\beta < \min\{\tilde{\delta} \frac{\log(2 - \gamma)}{d + \log(2 - \gamma)}, \sqrt{1 + \tilde{\delta}^2/2} - 1\}$ then there exists an extension of $\int_U \tilde{\alpha}_n(\cdot, \mathbf{y}_s, \mathbf{0})$, for $n = 1, \dots, N_f$, which is holomorphic on Θ_{β, N_s} .*

Proof. Consider the extension of $\mathbf{y}_s \rightarrow \mathbf{z}_s$, where $\mathbf{z}_s \in \mathbb{C}^{N_s}$. We first show that

$$(18) \quad \int_U \nabla(\tilde{u} \circ F)(\mathbf{y}_s, \mathbf{y}_f))^T \partial_{\tilde{y}_n^f} G(\mathbf{y}_s, \mathbf{y}_f) \nabla \varphi(\mathbf{y}_s, \mathbf{y}_f)$$

for $n = 1, \dots, N_f$ can be extended on Θ_{β, N_s} . Note that for the sake of reducing notation clutter we dropped the dependence of the variable $x \in U$ and it is understood from context unless clarification is needed.

We now show that each entry of the matrix $\partial_{\tilde{y}_n^f} G(\mathbf{z}_s, \mathbf{y}_f)$ is holomorphic on Θ_{β, N_s} for all $\mathbf{y} \in \Gamma_f$. First, we have that

$$\begin{aligned} \partial_{\tilde{y}_n^f} G(\mathbf{z}_s, \mathbf{y}_f) &= (\partial_{\tilde{y}_n^f} (a \circ F)(\mathbf{z}_s, \mathbf{y}_f)) C^{-1}(\mathbf{z}_s, \mathbf{y}_f) \det(\partial F(\mathbf{z}_s, \mathbf{y}_f)) \\ &\quad + (a \circ F)(\mathbf{z}_s, \mathbf{y}_f) \left(C^{-1}(\mathbf{z}_s, \mathbf{y}_f) \partial_{\tilde{y}_n^f} \det(\partial F(\mathbf{z}_s, \mathbf{y}_f)) \right. \\ &\quad \left. + \det(\partial F(\mathbf{z}_s, \mathbf{y}_f)) \partial_{\tilde{y}_n^f} C^{-1}(\mathbf{z}_s, \mathbf{y}_f) \right). \end{aligned}$$

From Assumption 5 $(a \circ F)(\cdot, \mathbf{z}_s)$ and $\partial_{\tilde{y}_i^f} (a \circ F)(\cdot, \mathbf{z}_s, \mathbf{y}_f) = 0$ are holomorphic on Θ_{β, N_s} for all $\mathbf{y}_f \in \Gamma_f$. From matrix calculus identities we have that

$$\partial_{\tilde{y}_i^f} C^{-1}(\mathbf{z}_s, \mathbf{y}_f) = -C^{-1}(\mathbf{z}_s, \mathbf{y}_f) \left(\partial C_{\tilde{y}_n^f}(\mathbf{z}_s, \mathbf{y}_f) \right) C^{-1}(\mathbf{z}_s, \mathbf{y}_f).$$

Since $\beta < \tilde{\delta}$ the series

$$\partial F^{-1}(\mathbf{z}_s, \mathbf{y}) = (I + R(\mathbf{z}_s, \mathbf{y}_f))^{-1} = I + \sum_{k=1}^{\infty} R(\mathbf{z}_s, \mathbf{y}_f)^k$$

is convergent for all $\mathbf{z}_s \in \Theta_\beta$ and for all $\mathbf{y}_f \in \Gamma_f$. It follows that each entry of $\partial F(\mathbf{z}_s, \mathbf{y})^{-1}$ and therefore $C(\mathbf{z}_s, \mathbf{y})^{-1}$ is holomorphic for all $\mathbf{z}_s \in \Theta_{\beta, N_s}$ and for all $\mathbf{y}_f \in \Gamma_f$. We have that $\det(\partial F(\mathbf{z}_s, \mathbf{y}_f))$ and $\partial C_{\tilde{y}_n^f}(\mathbf{z}_s, \mathbf{y}_f)$ are functions of a finite polynomial therefore they are holomorphic for all $\mathbf{z}_s \in \Theta_{\beta, N_s}$ and $\mathbf{y}_f \in \Gamma_f$.

From Jacobi's formula we have that for all $\mathbf{z}_s \in \Theta_{\beta, N_s}$ and $\mathbf{y}_f \in \Gamma_f$

$$\begin{aligned} \partial_{\tilde{y}_n^f} \det(\partial F(\mathbf{z}_s, \mathbf{y}_f)) &= \text{tr}(\text{Adj}(\partial F(\mathbf{z}_s, \mathbf{y}_f)) \partial_{\tilde{y}_n^f} \partial F(\mathbf{z}_s, \mathbf{y}_f)) \\ &= \det(\partial F(\mathbf{z}_s, \mathbf{y}_f)) \text{tr}(\partial F(\mathbf{z}_s, \mathbf{y}_f)^{-1} B_n^f(x)). \end{aligned}$$

It follows that for all $\mathbf{z}_s \in \Theta_{\beta, N_s}$ and $\mathbf{y}_f \in \Gamma_f$ $\partial_{\tilde{y}_n^f} G(\mathbf{z}_s, \mathbf{y}_f)$ are holomorphic.

We shall now prove the main result. First, extend \mathbf{y}_s along the n^{th} dimension as $y_n \rightarrow z_n$, $z_n \in \mathbb{C}$ and let $\tilde{\mathbf{z}}_s = [z_1, \dots, z_{n-1}, z_{n+1}, \dots, z_{N_s}]$. From Theorem 1 we have that $(\tilde{u} \circ F)(\mathbf{z}_s, \mathbf{y}_f)$ and $\varphi(\mathbf{z}_s, \mathbf{y}_f)$ are holomorphic for $\mathbf{z}_s \in \Theta_{\beta, N_s}$ and $\mathbf{y}_f \in \Gamma_f$ if

$$\beta < \min\left\{\tilde{\delta} \frac{\log(2-\gamma)}{d + \log(2-\gamma)}, \sqrt{1 + \tilde{\delta}^2/2} - 1\right\}.$$

Thus from Theorem 1.9.1 in [9] the series

$$(\tilde{u} \circ F)(\cdot, \mathbf{z}_s, \mathbf{y}_f) = \sum_{l=0}^{\infty} \tilde{u}_l(\cdot, \tilde{\mathbf{z}}_s, \mathbf{y}_f) z_n^l \quad \text{and} \quad \varphi(\mathbf{z}_s, \mathbf{y}_f) = \sum_{l=0}^{\infty} \tilde{\varphi}_l(\cdot, \tilde{\mathbf{z}}_s, \mathbf{y}_f) z_n^l,$$

are absolutely convergent in $H_0^1(U)$ for all $z \in \mathbb{C}$, where $\tilde{u}_l(\cdot, \tilde{\mathbf{z}}_s, \mathbf{y}_f)$, $\tilde{\varphi}_l(\cdot, \tilde{\mathbf{z}}_s, \mathbf{y}_f) \in H_0^1(U)$ for $l = 0, \dots, \infty$. Furthermore,

$$\begin{aligned} \|\nabla(\tilde{u} \circ F)(\cdot, \mathbf{z}_s, \mathbf{y}_f)\|_{L^2(U)} &\leq \sum_{l=0}^{\infty} \|\nabla \tilde{u}_l(\cdot, \tilde{\mathbf{z}}_s, \mathbf{y}_f)\|_{L^2(U)} |z_n|^l \\ &\leq \sum_{l=0}^{\infty} \|\tilde{u}_l(\cdot, \tilde{\mathbf{z}}_s, \mathbf{y}_f)\|_{H_0^1(U)} |z_n|^l \end{aligned}$$

i.e. $\nabla(\tilde{u} \circ F)(\cdot, \mathbf{z}_s, \mathbf{y}_f)$ is holomorphic on Θ_{β, N_s} along the n^{th} dimension. A similar argument is made for $\nabla \varphi(\cdot, \mathbf{z}_s, \mathbf{y}_f)$.

Since the matrix $\partial_{\tilde{y}_n^f} G(\mathbf{z}_s, \mathbf{y}_f)$ is holomorphic for all $\mathbf{z}_s \in \Theta_{\beta, N_s}$ and $\mathbf{y}_f \in \Gamma_f$ then we can rewrite the (i, j) entry as $\sum_{k=0}^{\infty} g_k^{i,j}(\cdot, \tilde{\mathbf{z}}_s, \mathbf{y}_f) z_n^k$ where $g_k^{i,j}(\cdot, \tilde{\mathbf{z}}_s, \mathbf{y}_f) \in L^\infty(U)$. For each $i, j = 1, \dots, d$ consider the map

$$\begin{aligned} T_{i,j} &:= \int_U \partial_{\tilde{y}_n^f} G(\mathbf{z}_s, \mathbf{y}_f)(i, j) \partial_{x_i} \tilde{u}(\cdot, \mathbf{z}_s, \mathbf{y}_f) \partial_{x_j} \varphi(\cdot, \mathbf{z}_s, \mathbf{y}_f) \\ &= \sum_{k,l,p=0}^{\infty} z_n^{k+l+p} \int_U g_k^{i,j}(\cdot, \tilde{\mathbf{z}}_s, \mathbf{y}_f) \partial_{x_i} \tilde{u}_l(\cdot, \tilde{\mathbf{z}}_s, \mathbf{y}_f) \partial_{x_j} \tilde{\varphi}_p(\cdot, \tilde{\mathbf{z}}_s, \mathbf{y}_f). \end{aligned}$$

For $i, j = 1, \dots, d$, for all $\mathbf{z}_s \in \Theta_{\beta, N_s}$ and $\mathbf{y}_f \in \Gamma_f$

$$\begin{aligned}
|T_{i,j}| &\leq \sum_{k,l,p=0}^{\infty} |z_n|^{k+l+p} \int_U |g_k^{i,j}(\cdot, \mathbf{z}_s, \mathbf{y}_f) \partial_{x_i} \tilde{u}_l(\cdot, \tilde{\mathbf{z}}_s, \mathbf{y}_f) \partial_{x_i} \varphi_p(\cdot, \tilde{\mathbf{z}}_s, \mathbf{y}_f)| \\
&\quad (\text{From Cauchy Schwartz it follows that}) \\
&\leq \sum_{k,l,p=0}^{\infty} |z_n|^{k+l+p} \|g_k^{i,j}(\cdot, \tilde{\mathbf{z}}_s, \mathbf{y}_f)\|_{L^\infty(U)} \|\partial_{x_i} \tilde{u}_l(\cdot, \tilde{\mathbf{z}}_s, \mathbf{y}_f)\|_{L^2(U)} \\
&\quad \|\partial_{x_i} \varphi_p(\cdot, \tilde{\mathbf{z}}_s, \mathbf{y}_f)\|_{L^2(U)} \\
&\leq \sum_{k,l,p=0}^{\infty} |z_n|^{k+l+p} \|g_k^{i,j}(\cdot, \tilde{\mathbf{z}}_s, \mathbf{y}_f)\|_{L^\infty(U)} \|\tilde{u}_l(\cdot, \tilde{\mathbf{z}}_s, \mathbf{y}_f)\|_{H_0^1(U)} \\
&\quad \|\varphi_p(\cdot, \tilde{\mathbf{z}}_s, \mathbf{y}_f)\|_{H_0^1(U)} < \infty.
\end{aligned}$$

Thus equation (18) can be analytically extended on Θ_{β, N_s} along the n^{th} dimensions for all $\mathbf{y}_f \in \Gamma_f$. Equation (18) can now be analytically extended on the entire domain Θ_{β, N_s} . Repeat the analytic extension of (18) for $n = 1, \dots, N_s$. From Hartog's Theorem it follows that (18) is continuous in Θ_{β, N_s} . From Osgood's Lemma it follows that (18) is holomorphic on Θ_{β, N_s} . Following a similar argument as for (18) we can analytically extended the rest of the terms of $\alpha_n(\cdot, \mathbf{y}_s, \mathbf{y}_f)$ on Θ_{β, N_s} for $n = 1, \dots, N_f$. \square

6. ERROR ANALYSIS

In this section we analyze the error between the exact QoI $Q(\mathbf{y}_s, \mathbf{y}_f)$ and the sparse grid hybrid perturbation approximation $\mathcal{S}_w^{m,g}[\hat{Q}_h(\mathbf{y}_s, \mathbf{y}_f)]$. With a slight abuse of notation by $\mathcal{S}_w^{m,g}[\hat{Q}_h(\mathbf{y}_s, \mathbf{y}_f)]$ we mean the two sparse grids approximations:

$$\mathcal{S}_w^{m,g}[\hat{Q}_h(\mathbf{y}_s, \mathbf{y}_f)] := \mathcal{S}_w^{m,g}[Q_h(\mathbf{y}_s, \mathbf{0})] + \sum_{n=1}^{N_f} \sqrt{\mu_{f,n}} y_n^f \mathcal{S}_w^{m,g} \left[\int_U \tilde{\alpha}_{n,h}(\cdot, \mathbf{y}_s, \mathbf{0}) \right],$$

where $\alpha_{n,h}(\cdot, \mathbf{y}_s, \mathbf{0})$, for $n = 1, \dots, N_f$, and $Q_h(\mathbf{y}_s, \mathbf{y}_f)$ are the finite element approximations of $\alpha_n(\cdot, \mathbf{y}_s, \mathbf{0})$ and $Q(\mathbf{y}_s, \mathbf{y}_f)$ respectively. It is easy to show that $\text{var}(Q(\mathbf{y}_s, \mathbf{y}_f)) - \text{var}(\mathcal{S}_w^{m,g}[\hat{Q}_h(\mathbf{y}_s, \mathbf{y}_f)])$ is equal to

$$\underbrace{\mathbb{E}[Q^2(\mathbf{y}_s, \mathbf{y}_f) - \mathcal{S}_w^{m,g}[\hat{Q}_h(\mathbf{y}_s, \mathbf{y}_f)]^2]}_{(I)} - \underbrace{(\mathbb{E}[Q(\mathbf{y}_s, \mathbf{y}_f)]^2 - \mathbb{E}[\mathcal{S}_w^{m,g}[\hat{Q}_h(\mathbf{y}_s, \mathbf{y}_f)]^2])}_{(II)}.$$

(I) Applying Jensen's inequality we have that

(19)

$$\begin{aligned}
|\mathbb{E}[Q^2(\mathbf{y}) - \mathcal{S}_w^{m,g}[\hat{Q}_h(\mathbf{y})]^2]| &\leq \|Q(\mathbf{y}) + \mathcal{S}_w^{m,g}[\hat{Q}_h(\mathbf{y})]\|_{L_\rho^\infty(\Gamma)} (\|Q(\mathbf{y}) - \hat{Q}(\mathbf{y})\|_{L_\rho^2(\Gamma)} \\
&\quad + \|\hat{Q}(\mathbf{y}) - \hat{Q}_h(\mathbf{y})\|_{L_\rho^1(\Gamma)} + \|\hat{Q}_h(\mathbf{y}) - \mathcal{S}_w^{m,g}[\hat{Q}_h(\mathbf{y})]\|_{L_\rho^2(\Gamma)}).
\end{aligned}$$

(II) Similarly, we have that

$$\begin{aligned}
|\mathbb{E}[Q(\mathbf{y}_s, \mathbf{y}_f)]^2 - \mathbb{E}[\mathcal{S}_w^{m,g}[\hat{Q}_h(\mathbf{y}_s, \mathbf{y}_f)]]^2| &\leq \|Q(\mathbf{y}) + \mathcal{S}_w^{m,g}[\hat{Q}_h(\mathbf{y})]\|_{L_\rho^1(\Gamma)} \\
&\quad \|\mathcal{S}_w^{m,g}[\hat{Q}_h(\mathbf{y}_s)]\|_{L_\rho^1(\Gamma)} \\
&\leq \|Q(\mathbf{y}) + \mathcal{S}_w^{m,g}[\hat{Q}_h(\mathbf{y})]\|_{L_\rho^1(\Gamma)} (\|Q(\mathbf{y}) - \hat{Q}(\mathbf{y})\|_{L_\rho^1(\Gamma)} + \|\hat{Q}(\mathbf{y}) - \hat{Q}_h(\mathbf{y})\|_{L_\rho^1(\Gamma)} \\
&\quad + \|\hat{Q}_h(\mathbf{y}) - \mathcal{S}_w^{m,g}[\hat{Q}_h(\mathbf{y})]\|_{L_\rho^1(\Gamma)})
\end{aligned}$$

Applying Jensen inequality

$$(20) \quad \begin{aligned} |\mathbb{E}[Q(\mathbf{y}_s, \mathbf{y}_f)]^2 - \mathbb{E}[\mathcal{S}_w^{m,g}[\hat{Q}_h(\mathbf{y}_s, \mathbf{y}_f)]]^2| &\leq \|Q(\mathbf{y}) + \mathcal{S}_w^{m,g}\hat{Q}_h(\mathbf{y})\|_{L_\rho^2(\Gamma)} \\ &(\|Q(\mathbf{y}) - \hat{Q}(\mathbf{y})\|_{L_\rho^2(\Gamma)} + \|\hat{Q}(\mathbf{y}) - \hat{Q}_h(\mathbf{y})\|_{L_\rho^1(\Gamma)} + \|\hat{Q}_h(\mathbf{y}) - \mathcal{S}_w^{m,g}\hat{Q}_h(\mathbf{y})\|_{L_\rho^2(\Gamma)}). \end{aligned}$$

Combining equations (19) and (20) we have that

$$\begin{aligned} |\text{var}(Q(\mathbf{y})) - \text{var}(\mathcal{S}_w^{m,g}[\hat{Q}_h(\mathbf{y})])| &\leq C_P \underbrace{\|Q(\mathbf{y}) - \hat{Q}(\mathbf{y})\|_{L_\rho^2(\Gamma)}}_{\text{Perturbation}} \\ &+ C_{PFE} \underbrace{\|\hat{Q}(\mathbf{y}) - \hat{Q}_h(\mathbf{y})\|_{L_\rho^1(\Gamma)}}_{\text{Finite Element}} + C_{PSG} \underbrace{\|\hat{Q}_h(\mathbf{y}) - \mathcal{S}_w^{m,g}[\hat{Q}_h(\mathbf{y})]\|_{L_\rho^2(\Gamma)}}_{\text{Sparse Grid}}. \end{aligned}$$

Similarly we have that the mean error satisfies the following bound:

$$\begin{aligned} |\mathbb{E}[Q(\mathbf{y}_s, \mathbf{y}_f) - \mathcal{S}_w^{m,g}[\hat{Q}_h(\mathbf{y}_s, \mathbf{y}_f)]]| &\leq \underbrace{\|Q(\mathbf{y}) - \hat{Q}(\mathbf{y})\|_{L_\rho^2(\Gamma)}}_{\text{Perturbation (I)}} \\ &+ \underbrace{\|\hat{Q}(\mathbf{y}) - \hat{Q}_h(\mathbf{y})\|_{L_\rho^1(\Gamma)}}_{\text{Finite Element (II)}} + \underbrace{\|\hat{Q}_h(\mathbf{y}) - \mathcal{S}_w^{m,g}[\hat{Q}_h(\mathbf{y})]\|_{L_\rho^2(\Gamma)}}_{\text{Sparse Grid (III)}}. \end{aligned}$$

Remark 9. For the case that probability distributions $\rho(\mathbf{y}_s)$ and $\rho(\mathbf{y}_f)$ are independent then the mean correction is exactly zero, thus the mean error would be bounded by the following terms

$$\begin{aligned} |\mathbb{E}[Q(\mathbf{y}_s, \mathbf{y}_f)] - \mathbb{E}[\mathcal{S}_w^{m,g}[Q_h(\mathbf{y}_s)]]| &\leq C_T \underbrace{\|Q(\mathbf{y}_s, \mathbf{y}_f) - Q(\mathbf{y}_s)\|_{L_\rho^2(\Gamma)}}_{\text{Truncation}} \\ &+ C_{FE} \underbrace{\|Q(\mathbf{y}_s) - Q_h(\mathbf{y}_s)\|_{L_\rho^1(\Gamma_s)}}_{\text{Finite Element}} + C_{SG} \underbrace{\|Q_h(\mathbf{y}_s) - \mathcal{S}_w^{m,g}[Q_h(\mathbf{y}_s)]\|_{L_\rho^2(\Gamma_s)}}_{\text{Sparse Grid}} \end{aligned}$$

for some positive constants C_T, C_{FE} and C_{SG} . We refer the reader to Section 5 in [5] for the definition of the constants and bounds of these errors.

6.1. Perturbation error. In this section we analyze the error term (I):

$$(21) \quad \|Q(\mathbf{y}_s, \mathbf{y}_f) - \hat{Q}(\mathbf{y}_s, \mathbf{y}_f)\|_{L_\rho^2(\Gamma)} = \|\mathcal{R}(\mathbf{y}_s, \delta\mathbf{y}_f)\|_{L_\rho^2(\Gamma)}$$

where $\mathbf{y}_f = \mathbf{y}_0^f + \delta\mathbf{y}_f$, $\mathbf{y}_0^f = \mathbf{0}$ and the remainder is equal to

$$(22) \quad \mathcal{R}(\mathbf{y}_s, \delta\mathbf{y}_f) := \frac{1}{2} D_{\mathbf{y}_f}^2 Q(\mathbf{y}_s + \theta\delta\mathbf{y}_f)(\delta\mathbf{y}_f, \delta\mathbf{y}_f)$$

for some $\theta \in (0, 1)$. From the approximation $\hat{Q}(\mathbf{y}_s, \mathbf{y}_f)$ in equation (11) and the expansion from (9) it is clear that

$$|Q(\mathbf{y}_s, \mathbf{y}_f) - \hat{Q}(\mathbf{y}_s, \mathbf{y}_f)| \leq \frac{1}{2} D_{\mathbf{y}_f}^2 Q(\mathbf{y}_s + \theta\delta\mathbf{y}_f)(\delta\mathbf{y}_f, \delta\mathbf{y}_f).$$

We shall now prove a series of lemmas that will be used to bound the perturbation error.

Recall from Remark 6 that we use the approximation given by equation (12)

$$\langle D_{\mathbf{y}}Q(\mathbf{y}_s, \mathbf{y}_0^f), \delta \mathbf{y}_0^f \rangle = \sum_{n=1}^{N_f} \sqrt{\mu_{f,n}} \delta \tilde{y}_n^f \int_U \tilde{\alpha}_n(x, \mathbf{y}_s, \mathbf{y}_0^f) dx$$

where the variable dependence is on $\tilde{y}_n^f = \sqrt{\mu_{f,n}} y_n^f$ instead of y_n^f for $n = 1, \dots, N_f$. This will allow an explicit dependence of the mean and variance error on decay parameters μ_n^f of the tail. To make the exposition clearer we use the following notation, let

$$\tilde{\mathbf{y}}_f := \begin{bmatrix} \tilde{y}_1^f \\ \vdots \\ \tilde{y}_{N_f}^f \end{bmatrix} = \begin{bmatrix} \sqrt{\mu_{f,1}} y_1^f \\ \vdots \\ \sqrt{\mu_{f,N_f}} y_{N_f}^f \end{bmatrix}, \tilde{\mathbf{y}} := \begin{bmatrix} \mathbf{y}_s \\ \tilde{\mathbf{y}}_f \end{bmatrix}$$

and for all $\mathbf{y}_f \in \Gamma_f$ we have that $\delta \tilde{\mathbf{y}}_f := \tilde{\mathbf{y}}_f$.

Lemma 6. *For all $n = 1, \dots, N_f$ and for all $\mathbf{y} \in \Gamma$*

$$\sup_{x \in U} \sigma_{max} \left(\partial_{\tilde{y}_n^f} \partial F^{-1}(\mathbf{y}) \right) \leq \sup_{x \in U} \|B_{f,n}(x)\|_2 \mathbb{F}_{min}^{-2}$$

Proof. From matrix calculus we have

$$\partial_{\tilde{y}_n^f} \partial F^{-1}(\mathbf{y}) = -\partial F^{-1}(\mathbf{y}) \left(\partial_{\tilde{y}_n^f} \partial F(\mathbf{y}) \right) \partial F^{-1}(\mathbf{y})$$

and also

$$\sigma_{max} \left(\partial_{\tilde{y}_n^f} \partial F(\mathbf{y}) \right) \leq \sigma_{max}(B_{f,n}(x)).$$

From Assumption 1 the result follows. \square

Lemma 7. *For all $\mathbf{y} \in \Gamma$*

$$\sup_{x \in U} |\partial_{\tilde{y}_n^f} \det(\partial F(\mathbf{y}))| \leq \sup_{x \in U} \mathbb{F}_{max}^d \mathbb{F}_{min}^{-1} \|B_{f,n}(x)\|_2 d$$

Proof. Using Jacobi's formula we have that for all $\mathbf{y} \in \Gamma$

$$\begin{aligned} \partial_{\tilde{y}_n^f} \det(\partial F(\mathbf{y})) &= \text{tr}(\text{Adj}(\partial F(\mathbf{y})) \partial_{\tilde{y}_n^f} \partial F(\mathbf{y})) \\ &= \det(\partial F(\mathbf{y})) \sum_{i=1}^d \lambda_i(\partial F(\mathbf{y})^{-1} B_{f,n}(x)), \end{aligned}$$

where $\lambda_i(\cdot)$ are the eigenvalues. \square

Lemma 8. *For all $n, m = 1, \dots, N_f$ and for all $\mathbf{y} \in \Gamma$*

$$\sup_{x \in U} \sigma_{max} \left(\partial_{\tilde{y}_n^f} \partial_{\tilde{y}_m^f} \partial F^{-1}(\mathbf{y}) \right) \leq \sup_{x \in U} 2 \mathbb{F}_{min}^{-3} \|B_{f,n}(x)\|_2 \|B_{f,m}(x)\|_2.$$

Proof. Using matrix calculus identities we have that

$$\begin{aligned} \partial F^{-1}(\mathbf{y}) &= \partial F^{-1}(\mathbf{y}) \left[\left(\partial_{\tilde{y}_m^f} \partial F(\mathbf{y}) \right) \partial F^{-1}(\mathbf{y}) \left(\partial_{\tilde{y}_n^f} \partial F(\mathbf{y}) \right) \right. \\ &\quad \left. + \left(\partial_{\tilde{y}_n^f} \partial F(\mathbf{y}) \right) \partial F^{-1}(\mathbf{y}) \left(\partial_{\tilde{y}_m^f} \partial F(\mathbf{y}) \right) \right] \partial F^{-1}(\mathbf{y}). \end{aligned}$$

Taking the triangular and multiplicative inequality, and following the same approach as Lemma 6 we obtain the desired result. \square

Lemma 9. For $n, m = 1, \dots, N_f$ for all $\mathbf{y} \in \Gamma$

$$\sup_{x \in U} \sigma_{\max} \left(\partial_{\tilde{y}_m^f} \partial_{\tilde{y}_n^f} |\partial F(\mathbf{y})| \right) \leq \sup_{x \in U} d(d+1) \mathbb{F}_{\max}^d \mathbb{F}_{\min}^{-2} \|B_{f,n}(x)\|_2 \|B_{f,m}(x)\|_2.$$

Proof. Using Jacobi's formula we have

$$\begin{aligned} \partial_{\tilde{y}_m^f} \partial_{\tilde{y}_n^f} &= \partial_{\tilde{y}_m^f} (\det(\partial F(\mathbf{y})) \text{tr}(\partial F(\mathbf{y})^{-1} B_{f,n}(x))) \sqrt{\mu_{f,n}} \\ &= \partial_{\tilde{y}_m^f} \det(\partial F(\mathbf{y})) \text{tr}(\partial F(\mathbf{y})^{-1} B_{f,n}(x)) \\ &\quad + \det(\partial F(\mathbf{y})) \text{tr}(\partial_{\tilde{y}_m^f} \partial F(\mathbf{y})^{-1} B_{f,n}(x)) \\ &= \det(\partial F(\mathbf{y})) \text{tr}(\partial F(\mathbf{y})^{-1} B_{f,m}(x)) \text{tr}(\partial F(\mathbf{y})^{-1} B_{f,n}(x)) \\ &\quad - \det(\partial F(\mathbf{y})) \text{tr}(\partial F(\mathbf{y})^{-1} B_{f,m}(x) \partial F(\mathbf{y})^{-1} B_{f,n}(x)). \end{aligned}$$

The result follows. \square

Lemma 10. For all $v, w \in H_0^1(U)$, $\theta \in (0, 1)$, $\mathbf{y}_s \in \Gamma_s$ and $\delta \mathbf{y}_f \in \Gamma_f$ we have that

$$\begin{aligned} & \left| \int_U (a \circ F)(\cdot, \mathbf{y}_s, \mathbf{0}) (\nabla v)^T \partial_{\tilde{y}_n^f} G(\mathbf{y}_s + \theta \delta \tilde{\mathbf{y}}_f) \nabla w \right| \leq \|v\|_{H_0^1(U)} \|w\|_{H_0^1(U)} a_{\max} \\ & \mathcal{B}(d, \mathbb{F}_{\min}, \mathbb{F}_{\max}, B_{f,n}), \end{aligned}$$

where

$$\mathcal{B}(d, \mathbb{F}_{\min}, \mathbb{F}_{\max}, B_{f,n}) := \sup_{x \in U} (d+2) \mathbb{F}_{\max}^d \mathbb{F}_{\min}^{-3} \|B_{f,n}(x)\|_2.$$

Proof. First we expand the partial derivative of $G(\mathbf{y})$ with respect to \tilde{y}_n^f :

$$\begin{aligned} \partial_{\tilde{y}_n^f} G(\mathbf{y}) &= \partial_{\tilde{y}_n^f} \partial F^{-T}(\mathbf{y}) \partial F^{-1}(\mathbf{y}) |\partial F(\mathbf{y})| + \partial F^{-T}(\mathbf{y}) \partial_{\tilde{y}_n^f} \partial F^{-1}(\mathbf{y}) |\partial F(\mathbf{y})| \\ &\quad + \partial F^{-T}(\mathbf{y}) \partial F^{-1}(\mathbf{y}) \partial_{\tilde{y}_n^f} |\partial F(\mathbf{y})|, \end{aligned}$$

From Lemmas 6, 7 and the triangular inequality we have that

$$\sup_{x \in U, \mathbf{y} \in \Gamma} \sigma_{\max} \left(\partial_{\tilde{y}_n^f} G(\mathbf{y}) \right) \leq (d+2) \mathbb{F}_{\max}^d \mathbb{F}_{\min}^{-3} \|B_{f,n}(x)\|_2.$$

\square

Lemma 11. For all $v, w \in H_0^1(U)$, $\theta \in (0, 1)$ and $\delta \mathbf{y}_f \in \Gamma_f$ we have that

$$\left| \int_U (a \circ F)(\cdot, \mathbf{y}_s) (\nabla w)^T \partial_{\tilde{y}_n^f} \partial_{\tilde{y}_m^f} G(\mathbf{y}_s + \theta \delta \tilde{\mathbf{y}}_f) \nabla v \right|$$

is less or equal to

$$\|v\|_{H_0^1(U)} \|w\|_{H_0^1(U)} a_{\max} 2(d+3) \mathbb{F}_{\min}^{-4} \mathbb{F}_{\max}^d \|B_{f,n}(x)\|_2 \|B_{f,m}(x)\|_2.$$

Proof. Using matrix calculus identities we have that for all $\mathbf{y} \in \Gamma$

$$\begin{aligned} \partial_{\tilde{y}_m^f} \partial_{\tilde{y}_n^f} G(\mathbf{y}) &= \partial_{\tilde{y}_m^f} \partial_{\tilde{y}_n^f} \partial F^{-T}(\mathbf{y}) \partial F^{-1}(\mathbf{y}) |\partial F(\mathbf{y})| \\ &\quad + \partial_{\tilde{y}_n^f} \partial F^{-T}(\mathbf{y}) \partial_{\tilde{y}_m^f} \partial F^{-1}(\mathbf{y}) |\partial F(\mathbf{y})| \\ &\quad + \partial_{\tilde{y}_n^f} \partial F^{-T}(\mathbf{y}) \partial F^{-1}(\mathbf{y}) \partial_{\tilde{y}_m^f} |\partial F(\mathbf{y})| \\ &\quad + \partial_{\tilde{y}_m^f} \partial F^{-T}(\mathbf{y}) \partial_{\tilde{y}_n^f} \partial F^{-1}(\mathbf{y}) |\partial F(\mathbf{y})| \\ &\quad + \partial F^{-T}(\mathbf{y}) \partial_{\tilde{y}_m^f} \partial_{\tilde{y}_n^f} \partial F^{-1}(\mathbf{y}) |\partial F(\mathbf{y})| \\ &\quad + \partial F^{-T}(\mathbf{y}) \partial_{\tilde{y}_n^f} \partial F^{-1}(\mathbf{y}) \partial_{\tilde{y}_m^f} |\partial F(\mathbf{y})| \\ &\quad + \partial_{\tilde{y}_m^f} \partial F^{-T}(\mathbf{y}) \partial F^{-1}(\mathbf{y}) \partial_{\tilde{y}_n^f} |\partial F(\mathbf{y})| \\ &\quad + \partial F^{-T}(\mathbf{y}) \partial_{\tilde{y}_m^f} \partial F^{-1}(\mathbf{y}) \partial_{\tilde{y}_n^f} |\partial F(\mathbf{y})| \\ &\quad + \partial F^{-T}(\mathbf{y}) \partial F^{-1}(\mathbf{y}) \partial_{\tilde{y}_m^f} \partial_{\tilde{y}_n^f} |\partial F(\mathbf{y})|. \end{aligned}$$

From Lemmas 6, 7, 8, 9, and the triangular inequality we have that for all $\mathbf{y} \in \Gamma$

$$\|\partial_{\tilde{y}_m^f} \partial_{\tilde{y}_n^f} G(\mathbf{y})\|_2 \leq \sup_{x \in U} (7 + 3d + 2\mathbb{F}_{\min}^{-1} \mathbb{F}_{\max}^{-d}) \mathbb{F}_{\min}^{-4} \mathbb{F}_{\max}^d \|B_{f,n}(x)\|_2 \|B_{f,m}(x)\|_2$$

□

Assumption 7. For all $\mathbf{y} \in \Gamma$ we assume that $(f \circ F)(\cdot, \mathbf{y}) \in H^2(U)$.

Lemma 12. For all $\mathbf{y}_s \in \Gamma_s$ and $\delta \mathbf{y}_f \in \Gamma$ we have that:
(a)

$$\begin{aligned} \|\nabla D_{\mathbf{y}_f} \tilde{u}(\cdot, \mathbf{y}_s, \mathbf{0})(\delta \mathbf{y}_f)\|_{L^2(U)} &\leq \frac{\sup_{x \in U} \sum_{n=1}^{N_f} \sqrt{\mu_{f,n}}}{a_{\min} \mathbb{F}_{\min}^d \mathbb{F}_{\max}^{-2}} \\ &\quad \left(\|(\tilde{u} \circ F)(\cdot, \mathbf{y}_s, \mathbf{0})\|_{H_0^1(U)} + \|\hat{\mathbf{w}}\|_{H^1(U)} a_{\max} (d+2) \mathbb{F}_{\max}^d \mathbb{F}_{\min}^{-3} \|B_{f,n}(x)\|_2 \right. \\ &\quad + \mathbb{F}_{\max}^d \mathbb{F}_{\min}^{-1} \|\hat{v}\|_{[L^\infty(U)]^d} \|b_{f,n}\|_{L^\infty(U)} C_P(U) \sqrt{d} \|(f \circ F)(\cdot, \mathbf{y}_s, \mathbf{0})\|_{H^1(U)} \\ &\quad \left. + d C_P(U) \|(f \circ F)(\cdot, \mathbf{y}_s, \mathbf{0})\|_{L^2(U)} \mathbb{F}_{\max}^d \mathbb{F}_{\min}^{-1} \|B_{f,n}(x)\|_2 \right) \end{aligned}$$

(b)

$$\begin{aligned} \|\nabla D_{\mathbf{y}_f} \varphi(\mathbf{y}_s, \mathbf{0})(\delta \mathbf{y}_f)\|_{L^2(U)} &\leq \frac{\sup_{x \in U} \sum_{n=1}^{N_f} \sqrt{\mu_{f,n}} \|\varphi(\mathbf{y}_s, \mathbf{0})\|_{H_0^1(U)} a_{\max} (d+2) \|B_{f,n}\|_2}{a_{\min} \mathbb{F}_{\min}^d \mathbb{F}_{\max}^{-2} \mathbb{F}_{\max}^{-d} \mathbb{F}_{\min}^3}. \end{aligned}$$

Proof. (a) From Lemma 2, Remark 5 & 6 we have that for any $v \in H_0^1(U)$ and for all $\mathbf{y}_s \in \Gamma_s$ and $\delta \mathbf{y}_f \in \Gamma$

$$\begin{aligned} &a_{\min} \mathbb{F}_{\min}^d \mathbb{F}_{\max}^{-2} \|\nabla D_{\mathbf{y}_f} \tilde{u}(\cdot, \mathbf{y}_s, \mathbf{0})(\delta \mathbf{y}_f)\|_{L^2(U)} \|\nabla v\|_{L^2(U)} \\ &\leq \sum_{n=1}^{N_f} \sqrt{\mu_{f,n}} \delta y_n^f \left| \int_U -\nabla(\tilde{u} \circ F)(\cdot, \mathbf{y}_s, \mathbf{0})^T \partial_{\tilde{y}_n^f} G(\mathbf{y}_s, \mathbf{0}) \nabla v \right. \\ &\quad + (\partial_{\tilde{y}_n^f} (f \circ F)(\cdot, \mathbf{y}_s, \mathbf{0})) |\partial F(\mathbf{y}_s, \mathbf{0})| v + (f \circ F)(\cdot, \mathbf{y}_s, \mathbf{0}) \partial_{\tilde{y}_n^f} |\partial F(\mathbf{y}_s, \mathbf{0})| v \\ &\quad \left. - (\nabla \hat{\mathbf{w}}(\cdot, \mathbf{y}_s, \mathbf{0}))^T \partial_{\tilde{y}_n^f} G(\mathbf{y}_s, \mathbf{0}) \nabla v - (\nabla \partial_{\tilde{y}_n^f} \hat{\mathbf{w}}(\cdot, \mathbf{y}_s, \mathbf{0}))^T G(\mathbf{y}_s, \mathbf{0}) \nabla v \right|. \end{aligned}$$

With the choice of $v = D_{\mathbf{y}_f} \tilde{u}(\cdot, \mathbf{y}_s, \mathbf{0})(\delta \mathbf{y}_f)$ and from Lemma 10 we have that

$$\begin{aligned} \|\nabla D_{\mathbf{y}_f} \tilde{u}(\cdot, \mathbf{y}_s, \mathbf{0})(\mathbf{y}_s, \delta \mathbf{y})\|_{L^2(U)} &\leq \frac{1}{a_{\min} \mathbb{F}_{\min}^d \mathbb{F}_{\max}^{-2} \|\nabla v\|_{L^2(U)}} \left(\right. \\ &\sum_{i=1}^N \sqrt{\mu_{f,n}} \delta y_n^f \left| \int_U -(\nabla(\tilde{u} \circ F)(\cdot, \mathbf{y}_s, \mathbf{0}))^T \partial_{\tilde{y}_n^f} G(\mathbf{y}_s, \mathbf{0}) \nabla v \right. \\ &+ \partial_{\tilde{y}_n^f} (f \circ F)(\cdot, \mathbf{y}_s, \mathbf{0}) |\partial F(\mathbf{y}_s, \mathbf{0})| v + (f \circ F)(\cdot, \mathbf{y}_s, \mathbf{0}) \partial_{\tilde{y}_n^f} |\partial F(\mathbf{y}_s, \mathbf{0})| v \\ &\left. \left. - (\nabla \mathbf{w}(\mathbf{y}_s, \mathbf{0}))^T \partial_{\tilde{y}_n^f} G(\mathbf{y}_s, \mathbf{0}) \nabla v - (\partial_{\tilde{y}_n^f} \nabla \mathbf{w}(\mathbf{y}_s, \mathbf{0}))^T G(\mathbf{y}_s, \mathbf{0}) \nabla v \right| \right). \end{aligned}$$

Now,

$$\begin{aligned} \left| \int_U \partial_{\tilde{y}_n^f} (f \circ F)(\cdot, \mathbf{y}_s, \mathbf{0}) |\partial F(\mathbf{y}_s, \mathbf{0})| v \right| &\leq \mathbb{F}_{\max}^d \int_U |\partial_{\tilde{y}_n^f} (f \circ F)(\cdot, \mathbf{y}_s, \mathbf{0})| v| \\ &\leq \mathbb{F}_{\max}^d C_P(U) \|\nabla v\|_{L^2(U)} \left\| \sum_{l=1}^d |\partial_{F_l} f \partial_{\tilde{y}_n^f} F_l| \right\|_{L^2(U)} \\ &\leq \mathbb{F}_{\max}^d C_P(U) \|\nabla v\|_{L^2(U)} \|\hat{v}\|_{[L^\infty(U)]^d} \|b_{f,n}\|_{L^\infty(U)} \\ &\|\nabla f \cdot \mathbf{1}\|_{L^2(U)}. \end{aligned}$$

From the Sobolev chain rule (see Theorem 3.35 in [1]) for any $v \in H^1(D(\omega))$ we have that $\nabla v = \partial F^{-T} \nabla(v \circ F)$, where $v \circ F \in H^1(U)$, thus

$$\begin{aligned} \|\nabla f \cdot \mathbf{1}\|_{L^2(U)} &= \|\mathbf{1}^T \partial F^{-T} \nabla(f \circ F)(\cdot, \mathbf{y}_s, \mathbf{0})\|_{L^2(U)} \\ &\leq \mathbb{F}_{\min}^{-1} \sqrt{d} \|\nabla(f \circ F)(\cdot, \mathbf{y}_s, \mathbf{0})\|_2 \| \mathbf{1} \|_{L^2(U)} \\ &\leq \mathbb{F}_{\min}^{-1} \sqrt{d} \|(f \circ F)(\cdot, \mathbf{y}_s, \mathbf{0})\|_{H^1(U)}. \end{aligned}$$

From Lemma 7 the result follows.

(b) Apply Lemma 3 with $v = D_{\mathbf{y}_f} \varphi(\mathbf{y}_s, \mathbf{0})(\delta \mathbf{y}_f)$ and we get the result. \square

Lemma 13. *For all $\mathbf{y} \in \Gamma$ and $n, m = 1, \dots, N$ we have that*

$$\begin{aligned} \|\partial \tilde{y}_n^f (f \circ F)(\cdot, \mathbf{y})\|_{L^2(U)} \\ \leq \mathbb{F}_{\min}^{-1} \sqrt{d} \|b_{f,n}\|_{L^\infty(U)} \|\hat{v}\|_{[L^\infty(U)]^d} \|(f \circ F)(\cdot, \mathbf{y})\|_{H^1(U)}. \end{aligned}$$

and

$$\begin{aligned} \partial \tilde{y}_n^f \partial y_m^f (f \circ F)(\cdot, \mathbf{y})\|_{L^2(U)} &\leq d \|b_{f,n}\|_{L^\infty(U)} \|b_{f,m}\|_{L^\infty(U)} \|\hat{v}\|_{[W^{1,\infty}(U)]^d}^2 \\ &(d \mathbb{F}_{\min}^{-2} (d^{3/2} \|f \circ F\|_{H^1(U)} \mathbb{F}_{\min}^{-2} (1 + 4 \|\hat{v}\|_{[L^\infty(U)]^d} \left(\sum_{i=1}^{N_s} \sqrt{\mu_{s,i}} \|b_{s,i}\|_{W^{2,\infty}(U)} \right. \\ &\left. + \sum_{i=1}^{N_f} \sqrt{\mu_{f,i}} \|b_{f,i}\|_{W^{2,\infty}(U)} \right)) + \|f \circ F\|_{H^2(U)}). \end{aligned}$$

Proof. The first bound is immediate. Follow the proof in Lemma 12 (a). Now, by applying the chain rule for Sobolev spaces we obtain that for all $\mathbf{y} \in \Gamma$

$$\begin{aligned}
 \|\partial \tilde{y}_n^f \partial \tilde{y}_m^f (f \circ F)(\cdot, \mathbf{y})\|_{L^2(U)} &= \|(b_m b_n (\sum_{i=1}^d \hat{v}_i \sum_{j=1}^d \hat{v}_j \partial_{F_i} \partial_{F_j} f))\|_{L^2(U)} \\
 (23) \quad &\leq d \|b_n\|_{L^\infty(U)} \|b_m\|_{L^\infty(U)} \|\hat{v}\|_{[L^\infty(U)]^d}^2 \\
 &\quad \sum_{i=1}^d \sum_{j=1}^d |\partial_{F_i} \partial_{F_j} f|
 \end{aligned}$$

Now,

$$(24) \quad \sum_{i=1}^d \sum_{j=1}^d |\partial_{F_i} \partial_{F_j} f| = \mathbf{1}^T \partial^2 f \mathbf{1},$$

where $\partial^2 f$ refers to the Hessian of f . From the Chain Rule for Hessians [19] and adapting for Sobolev spaces [1] we obtain

$$\partial^2 (f \circ F) = \partial F \partial^2 f \partial F^T + \nabla f \star \mathcal{H},$$

where $\partial^2 f$ refers to the Hessian of f ,

$$\nabla f \star \mathcal{H} := \begin{bmatrix} (\nabla f)^T \mathcal{H}_{1,1} & \dots & (\nabla f)^T \mathcal{H}_{1,d} \\ \vdots & \ddots & \vdots \\ (\nabla f)^T \mathcal{H}_{d,1} & \dots & (\nabla f)^T \mathcal{H}_{d,d} \end{bmatrix}$$

and

$$\mathcal{H}_{i,j} := \begin{bmatrix} \partial_{x_i} \partial_{x_j} F_1 \\ \vdots \\ \partial_{x_i} \partial_{x_j} F_d \end{bmatrix}$$

for all $i, j = 1, \dots, d$. It follows that

$$(25) \quad |\mathbf{1}^T \partial^2 f \mathbf{1}| \leq d \mathbb{F}_{min}^{-2} (\|\partial^2 (f \circ F)\|_2 + \|\nabla f \star \mathcal{H}\|_2).$$

Furthermore,

$$\begin{aligned}
 \|\nabla f \star \mathcal{H}\|_2 &\leq \|\nabla f \star \mathcal{H}\|_F \leq \sqrt{\sum_{i,j=1}^d |(\nabla f)^T \partial F(\mathbf{y})^{-1} \mathcal{H}_{i,j}|^2} \\
 (26) \quad &\leq \|\nabla f\|_2 \mathbb{F}_{min}^{-1} \sqrt{\sum_{i,j=1}^d \|\mathcal{H}_{i,j}\|_2^2} \\
 &\leq d^{3/2} \|\partial F^{-T} \nabla (f \circ F)\|_2 \mathbb{F}_{min}^{-1} \sup_{i,j,n} |\partial_{x_i} \partial_{x_j} F_n| \\
 &\leq d^{3/2} \|(f \circ F)\|_{H^1(U)} \mathbb{F}_{min}^{-2} \sup_{i,j,n} |\partial_{x_i} \partial_{x_j} F_n|
 \end{aligned}$$

Now, for $i, j = 1, \dots, N$ we have

$$(27) \quad |\partial_{x_i} \partial_{x_j} F_n| \leq 1 + 4 \|\hat{v}\|_{[W^{1,\infty}(U)]^d} \sum_{n=1}^N \sqrt{\mu_n} \|b_n\|_{W^{2,\infty}(U)}.$$

Combining (23), (24), (25), (26) and (27) we obtain the result. \square

From Lemmas 5 and 6 - 13 we have that for all $\mathbf{y}_s \in \Gamma_s$ and for all $\delta \mathbf{y}_f \in \Gamma_f$

$$|D_{\mathbf{y}_f}^2 Q(\mathbf{y})(\delta \mathbf{y}_f, \delta \mathbf{y}_f)| \leq \sum_{n,m=1}^{N_f} |\delta \tilde{y}_n^f| |\delta \tilde{y}_m^f| G_{n,m},$$

where

$$\begin{aligned} & G_{n,m} (\| (f \circ F)(\mathbf{y}_s, \mathbf{0}) \|_{H^2(U)}, \| (\tilde{u} \circ F)(\mathbf{y}_s, \mathbf{0}) \|_{H^1(U)}, C_P(U), \\ & \| \varphi(\mathbf{y}_s, \mathbf{0}) \|_{H^1(U)}, \| \mathbf{w}(\mathbf{y}_s, \mathbf{0}) \|_{H^1(U)}, \| B_{f,n} \|_2, \| B_{f,m} \|_2, \| b_{f,m} \|_{W^{2,\infty}(U)}, \\ & \| b_{f,n} \|_{W^{2,\infty}(U)}, a_{\max} \mathbb{F}_{\max}, \mathbb{F}_{\min}, d, \| \hat{v} \|_{[W^{2,\infty}(U)]^d}, \sum_{l=1}^N \sqrt{\mu_{s,l}} \| b_{s,l} \|_{W^{2,\infty}(U)} \\ & , \sum_{l=1}^N \sqrt{\mu_{f,l}} \| b_{f,l} \|_{W^{2,\infty}(U)}) \end{aligned}$$

is a bounded constant that depends on the indicated parameters. We have now proven the following result.

Theorem 3. For all $\mathbf{y}_s \in \Gamma_s$ and $\mathbf{y}_f \in \Gamma_f$

$$\| Q(\mathbf{y}_s, \mathbf{y}_f) - \hat{Q}(\mathbf{y}_s, \mathbf{y}_f) \|_{L_\rho^2(\Gamma)} \leq \frac{1}{2} \sum_{n,m=1}^{N_f} \sqrt{\mu_{f,n}} \sqrt{\mu_{f,m}} G_{n,m} \leq \mathbb{G} \left(\sum_{k=1}^{N_f} \sqrt{\mu_{f,k}} \right)^2,$$

where $\mathbb{G} := \frac{1}{2} \sup_{n,m} G_{n,m}$.

6.2. Finite element error. The finite element convergence rate is directly depend on the regularity of the solution u and influence function φ , the polynomial order $H_h(U) \subset H_0^1(U)$ of the finite element space and the mesh size h). By applying the triangular and Jensen inequalities we obtain

$$\begin{aligned} & \| \hat{Q}(\mathbf{y}_s, \mathbf{y}_f) - \hat{Q}_h(\mathbf{y}_s, \mathbf{y}_f) \|_{L_\rho^1(\Gamma)} \leq \| Q(\mathbf{y}_s, \mathbf{0}) - Q_h(\mathbf{y}_s, \mathbf{0}) \|_{L_\rho^1(\Gamma_s)} \\ & + \sum_{n=1}^{N_f} \sqrt{\mu_{f,n}} \left\| \int_U \tilde{\alpha}_n(x, \mathbf{y}_s, \mathbf{0}) - \tilde{\alpha}_{i,h}(x, \mathbf{y}_s, \mathbf{0}) \right\|_{L_\rho^2(\Gamma_s)}. \end{aligned}$$

Following a duality argument we obtain

$$\| Q(\mathbf{y}_s, \mathbf{0}) - Q_h(\mathbf{y}_s, \mathbf{0}) \|_{L_\rho^1(\Gamma_s)} \leq a_{\max} \mathbb{F}_{\max}^d \mathbb{F}_{\min}^{-2} C_{\Gamma_s}(r) D_{\Gamma_s}(r) h^{2r}.$$

for some constant $r \in \mathbb{N}$, $C_{\Gamma_s}(r) := \int_{\Gamma_s} C(r, u(\mathbf{y}_s, \mathbf{0})) \rho(\mathbf{y}_s) d\mathbf{y}$ and $D_{\Gamma_s}(r) := \int_{\Gamma_s} C(r, \varphi(\mathbf{y}_s, \mathbf{0})) \rho(\mathbf{y}_s) d\mathbf{y}$. The constant r depends on the polynomial degree of the finite element basis and the regularity properties of the solution $\tilde{u} \circ F$ (which is dependent on the regularity of f , the diffusion coefficient a and the mapping F). It follows that

$$(28) \quad \| \hat{Q}(\mathbf{y}_s, \mathbf{0}) - \hat{Q}_h(\mathbf{y}_s, \mathbf{0}) \|_{L_\rho^2(\Gamma)} \leq \mathbb{S}_0 h^{2r} + h^r \sum_{n=1}^{N_f} \mathbb{S}_n \sqrt{\mu_{f,n}}$$

where $\mathbb{S}_0 := a_{\max} \mathbb{F}_{\max}^d \mathbb{F}_{\min}^{-2} C_{\Gamma_s}(r) D_{\Gamma_s}(r)$ and

$$\begin{aligned} & \mathbb{S}_n (\| (f \circ F)(\mathbf{y}_s, \mathbf{0}) \|_{L^2(U)}, \| \mathbf{w}(\mathbf{y}_s, \mathbf{0}) \|_{H^1(U)}, \| B_{f,n} \|_2, \| b_{f,n} \|_{L^\infty(U)}, \\ & a_{\max} \mathbb{F}_{\max}, \mathbb{F}_{\min}, d, \| \hat{v} \|_{[L^\infty(U)]^d}, C_{\Gamma_s}(r), D_{\Gamma_s}(r)) \end{aligned}$$

are bounded constants for $n = 1, \dots, N_f$.

6.3. Sparse grid error. For the sake of simplicity, we will only explicitly show the convergence rates for the isotropic Smolyak sparse grid. However, this analysis can be extended to the anisotropic case without much difficulty. Now, we have that

$$\begin{aligned} \|\hat{Q}_h(\mathbf{y}_s, \mathbf{y}_f) - \mathcal{S}_w^{m,g} \hat{Q}_h(\mathbf{y}_s, \mathbf{y}_f)\|_{L_\rho^2(\Gamma)} &\leq a_{max} \mathbb{F}_{max}^d \mathbb{F}_{min}^{-2} \|e_0\|_{L_\rho^2(\Gamma_s; H_0^1(U))} \\ &+ \sum_{n=1}^{N_f} \sqrt{\mu_{f,i}} \|e_n\|_{L_\rho^2(\Gamma_s)}, \end{aligned}$$

where $e_0 := \hat{u}_h(\mathbf{y}_s, \mathbf{0}) - \mathcal{S}_w^{m,g}[\hat{u}_h(\mathbf{y}_s, \mathbf{0})]$ and

$$e_n := \int_U \tilde{\alpha}_{n,h}(\mathbf{y}_s, \mathbf{0}) - \mathcal{S}_w^{m,g}[\int_U \tilde{\alpha}_{n,h}(\mathbf{y}_s, \mathbf{0})]$$

for $n = 1, \dots, N_f$, and

$$L_\rho^q(\Gamma_s; V) := \{v : \Gamma_s \times U \rightarrow V \text{ is strongly measurable, } \int_\Gamma \|v\|_V^q \rho(\mathbf{y}) d\mathbf{y} < \infty\}.$$

for any Banach space V defined on U .

In [17, 18] the error estimates for isotropic and anisotropic Smolyak sparse grids with Clenshaw-Curtis and Gaussian abscissas are derived. It is shown that $\|e_0\|_{L_\rho^2(\Gamma_s; H_0^1(U))}$ (and $\|e_n\|_{L_\rho^2(\Gamma_s)}$ for $n = 1, \dots, N_f$) exhibit algebraic or sub-exponential convergence with respect to the number of collocation knots η . For these estimates to be valid it is assumed that the semi-discrete solution $\hat{u}_{0,h} := \hat{u}_h(\mathbf{y}_s, \mathbf{0})$ and $\hat{u}_{n,h} := \int_U \tilde{\alpha}_{k,n}(\cdot, \mathbf{y}_s, \mathbf{0})$, $n = 1, \dots, N_f$ admit an analytic extension in the same region Θ_{β, N_s} . This is a reasonable assumption to make.

Consider the polyellipse in $\mathcal{E}_{\sigma_1, \dots, \sigma_{N_s}} := \Pi_{n=1}^{N_s} \mathcal{E}_{n, \sigma_n} \subset \mathbb{C}^{N_s}$ where

$$\begin{aligned} \mathcal{E}_{n, \sigma_n} &:= \left\{ z \in \mathbb{C}; \sigma_n > 0; \sigma_n \geq \kappa_n \geq 0; \operatorname{Re}(z) = \frac{e^{\kappa_n} + e^{-\kappa_n}}{2} \cos(\theta), \right. \\ &\quad \left. \operatorname{Im}(z) = \frac{e^{\kappa_n} - e^{-\kappa_n}}{2} \sin(\theta), \theta \in [0, 2\pi) \right\}, \end{aligned}$$

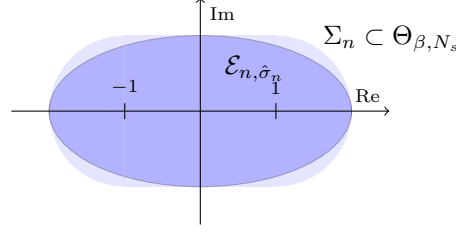
and

$$\Sigma_n := \left\{ z_n \in \mathbb{C}; y_n = y + w_n, y \in [-1, 1], |w_n| \leq \tau_n := \frac{\beta}{1 - \delta} \right\}$$

for $n = 1, \dots, N_s$. For the sparse grid error estimates to be valid the solution $(\tilde{u}_h(\cdot, \mathbf{y}_s, \mathbf{0})$ and $\int_U \tilde{\alpha}_{n,h}(\cdot, \mathbf{y}_s, \mathbf{0})$, $n = 1, \dots, N_f$, have to admit an extension on the polyellipse $\mathcal{E}_{\sigma_1, \dots, \sigma_{N_s}}$. The coefficients σ_n , for $n = 1, \dots, N$ control the overall decay $\hat{\sigma}$ of the sparse grid error estimate. Since we restrict our attention to isotropic sparse grids the decay will be dictated by the smallest σ_n i.e. $\hat{\sigma} \equiv \min_{n=1, \dots, N_s} \sigma_n$.

The next step is to find a suitable embedding of $\mathcal{E}_{\sigma_1, \dots, \sigma_{N_s}}$ in Θ_{β, N_s} . Thus we need to pick the largest σ_n , $n = 1, \dots, N_s$ such that $\mathcal{E}_{\sigma_1, \dots, \sigma_{N_s}} \subset \Theta_{\beta, N_s}$. This is achieved by forming the set $\Sigma := \Sigma_1 \times \dots \times \Sigma_{N_s}$ and letting $\sigma_1 = \sigma_2 = \dots = \sigma_{N_s} = \hat{\sigma} = \log(\sqrt{\tau_{N_s}^2 + 1} + \tau_{N_s}) > 0$ as shown in Figure 2.

We now have almost everything we need to state the sparse grid error estimates. However, in [18] to simplify the estimate it is assumed that if $v \in C^0(\Gamma; H_0^1(U))$ then the term $M(v)$ (see page 2322) is equal to one. We reintroduce the term $M(v)$ and note that it can be bounded by $\max_{\mathbf{z} \in \Theta_{\beta, N_s}} \|v(\mathbf{z})\|_{H_0^1(U)}$ and update the sparse grids error estimate. To this end let $\tilde{M} := \max_{n=0}^{N_s} \max_{\mathbf{z} \in \Theta_{N_s, \beta}} \|\tilde{u}_{n,h}(\mathbf{z})\|_{H_0^1(U)}$.

FIGURE 2. Embedding of $\mathcal{E}_{n, \hat{\sigma}_n}$ in $\Sigma_n \subset \Theta_{\beta, N_s}$.

Remark 10. In [5] Corollary 8 a bound for $\|\hat{u}(\cdot, \mathbf{z})\|_{H_0^1(U)}$, $\mathbf{z} \in \Theta_{\beta, N_s}$, can be obtained by applying the Poincaré inequality. Following a similar argument a bound for $\|\hat{\varphi}(\cdot, \mathbf{z})\|_{H_0^1(U)}$ for all $\mathbf{z} \in \Theta_{\beta, N_s}$. Thus bounds for $\|\tilde{u}_{n,h}(\mathbf{z})\|_{H_0^1(U)}$ for $n = 0, \dots, N_s$ and for all $\mathbf{z} \in \Theta_{\beta, N_s}$ can be obtained.

Modifying Theorem 3.11 in [18] it can be shown that given a sufficiently large η ($w > N_s/\log 2$) a Smolyak sparse grid with a nested Clenshaw Curtis abscissas we obtain the following estimate

$$(29) \quad \|e_n\|_{L_\rho^2(\Gamma_s)} \leq \mathcal{Q}(\sigma, \delta^*(\sigma), N_s, \tilde{M}) \eta^{\mu_3(\sigma, \delta^*, N_s)} \exp\left(-\frac{N_s \sigma}{2^{1/N_s}} \eta^{\mu_2(N_s)}\right)$$

for $n = 0, \dots, N_f$, where $\sigma = \hat{\sigma}/2$, $\delta^*(\sigma) := (e \log(2) - 1)/\tilde{C}_2(\sigma)$,

$$\mathcal{Q}(\sigma, \delta^*(\sigma), N_s, \tilde{M}) := \frac{C_1(\sigma, \delta^*(\sigma), \tilde{M})}{\exp(\sigma \delta^*(\sigma) \tilde{C}_2(\sigma))} \frac{\max\{1, C_1(\sigma, \delta^*(\sigma), \tilde{M})\}^{N_s}}{|1 - C_1(\sigma, \delta^*(\sigma), \tilde{M})|},$$

$\mu_2(N_s) = \frac{\log(2)}{N_s(1+\log(2N_s))}$ and $\mu_3(\sigma, \delta^*(\sigma), N_s) = \frac{\sigma \delta^*(\sigma) \tilde{C}_2(\sigma)}{1+\log(2N_s)}$. Furthermore, $C(\sigma) = \frac{4}{e^{2\sigma}-1}$,

$$\tilde{C}_2(\sigma) = 1 + \frac{1}{\log 2} \sqrt{\frac{\pi}{2\sigma}}, \quad \delta^*(\sigma) = \frac{e \log(2) - 1}{\tilde{C}_2(\sigma)},$$

$$C_1(\sigma, \delta, \tilde{M}) = \frac{4\tilde{M}C(\sigma)a(\delta, \sigma)}{e\delta\sigma},$$

and

$$a(\delta, \sigma) := \exp\left(\delta\sigma \left\{ \frac{1}{\sigma \log^2(2)} + \frac{1}{\log(2)\sqrt{2\sigma}} + 2 \left(1 + \frac{1}{\log(2)} \sqrt{\frac{\pi}{2\sigma}}\right) \right\}\right).$$

7. COMPLEXITY AND TOLERANCE

In this section we derive the total work W needed such that $|\text{var}[Q(\mathbf{y}_s, \mathbf{y}_f)] - \text{var}[\mathcal{S}_w^{m,g}[\hat{Q}_h(\mathbf{y}_s, \mathbf{y}_f)]]|$ and $|\mathbb{E}[Q(\mathbf{y}_s, \mathbf{y}_f)] - \mathbb{E}[\mathcal{S}_w^{m,g}[\hat{Q}_h(\mathbf{y}_s, \mathbf{y}_f)]]|$ for the isotropic CC sparse grid is less or equal to a given tolerance parameter $\text{tol} \in \mathbb{R}^+$.

Let N_h be the number of degrees of freedom used to compute the semi-discrete approximation $u_h \in H_h(U) \subset H_0^1(U)$. We assume that the computational complexity for solving u_h is $\mathcal{O}(N_h^q)$ for each realization, where the constant $q \geq 1$ reflects the optimality of the finite element solver. The cost for solving the approximation of the influence function $\varphi_h \in H_h(U)$ is also $\mathcal{O}(N_h^q)$. Thus for any $\mathbf{y}_s \in \Gamma_s$, the cost for computing $Q_h(\mathbf{y}_s, \mathbf{0}) := B(\mathbf{y}_s, \mathbf{0}; u_h(\mathbf{y}_s, \mathbf{0}), \varphi_h(\mathbf{y}_s, \mathbf{0}))$ is bounded by

$\mathcal{O}(N_h d^2 + N_h^q)$. Similarly, for any $\mathbf{y}_s \in \Gamma_s$ the cost for evaluating $\int_U \tilde{\alpha}_{n,h}(\cdot, \mathbf{y}_s, \mathbf{0})$ is $\mathcal{O}(N_h d^2 + N_h^q)$.

Remark 11. *To compute the expectation integrals for the mean and variance correction a Gauss quadrature scheme coupled with an auxiliary probability distribution $\hat{\rho}(\mathbf{y})$ such that*

$$\hat{\rho}(\mathbf{y}) = \Pi_{n=1}^N \rho_n(y_n) \text{ and } \rho/\hat{\rho} < C < \infty.$$

for some $C > 0$ (See [5] for details). However, to simplify the analysis it is assumed that quadrature is exact and of cost $\mathcal{O}(1)$.

Let $\mathcal{S}_w^{m,g}$ be the sparse grid operator characterized by $m(i)$ and $g(\mathbf{i})$. Furthermore, let $\eta_0(N_s, m, g, w, \Theta_{\beta, N_s})$ be the number of the sparse grid knots for constructing $\mathcal{S}_w^{m,g}[\tilde{\alpha}_{n,h}(\cdot, \mathbf{y}_s, \mathbf{0})]$ and $\eta_n(N_s, m, g, w, \Theta_{\beta, N_s})$ for constructing $\mathcal{S}_w^{m,g}[\tilde{\alpha}_{n,h}(\cdot, \mathbf{y}_s, \mathbf{0})]$, for $n = 1, \dots, N_f$. The cost for computing $\mathbb{E}[\mathcal{S}_w^{m,g}[Q_h(\mathbf{y}_s, \mathbf{0})]]$ is $\mathcal{O}((N_h d^2 + N_h^q)\eta_0)$ and the cost for computing $\sum_{n=1}^{N_f} \sqrt{\mu_{f,n}} \mathbb{E}[\tilde{y}_n^f \mathcal{S}_w^{m,g}[\int_U \tilde{\alpha}_n(\cdot, \mathbf{y}_s, \mathbf{0})]]$ is bounded by $\mathcal{O}((N_h d^2 + N_h^q)N_f \eta)$, where

$$\eta := \max_{n=0, \dots, N_f} \eta_n.$$

The total cost for computing the mean correction is bounded by

$$(30) \quad W_{Total}^{mean}(tol) = \mathcal{O}((N_h(tol)d^2 + N_h^q(tol))N_f(tol)\eta(tol)).$$

Following a similar argument the cost for computing the variance correction is bounded by

$$(31) \quad W_{Total}^{var}(tol) = \mathcal{O}((N_h(tol)d^2 + N_h^q(tol))N_f^2(tol)\eta(tol)).$$

We now obtain the estimates for $N_h(tol)$, $N_f(tol)$ and $\eta(tol)$ for the Perturbation, Finite Element and Sparse Grids respectively:

(a) **Perturbation:** From the truncation estimate derived in Section 6.1 we seek $\|Q(\mathbf{y}_s, \mathbf{y}_f) - \hat{Q}(\mathbf{y}_s, \mathbf{y}_f)\|_{L_\rho^2(\Gamma)} \leq \frac{tol}{3C_P}$ with respect to the decay of the coefficients $\sqrt{\mu_{f,n}}$, $n = 1, \dots, N_f$. First, make the assumption that $B_T := \sum_{n=1}^{N_f} \sqrt{\mu_{f,n}} \leq C_D N_s^{-l}$ for some uniformly bounded $C_D > 0$ and $l > 0$. It follows that $\|Q(\mathbf{y}_s, \mathbf{y}_f) - \hat{Q}(\mathbf{y}_s, \mathbf{y}_f)\|_{L_\rho^2(\Gamma)} \leq \frac{tol}{3C_P}$ if

$$B_T^2 \mathbb{G} \leq C_D^2 N_s^{-2l} \mathbb{G} \leq \frac{tol}{3C_P}.$$

Finally, we have that

$$N_f(tol) \geq \left(\frac{tol}{3C_P C_D^2 \mathbb{G}} \right)^{-1/(2l)}.$$

(b) **Finite Element:** From Section 6.2 if

$$\mathbb{S}_0 h^{2r} + B_T \mathbb{T}_0 h^r \leq \frac{tol}{3C_{PFE}},$$

$\mathbb{T}_0 := \max_{n=1}^{N_f} \mathbb{S}_n$, then $\|\hat{Q}(\mathbf{y}_s, \mathbf{0}) - \hat{Q}_h(\mathbf{y}_s, \mathbf{0})\|_{L_\rho^2(\Gamma; H_0^1(U))} \leq \frac{tol}{3C_{PFE}}$. Solving the quadratic inequality we obtain that

$$h(tol) \leq \left(-\frac{B_T \mathbb{T}_0}{2\mathbb{S}_0} + \left(\left(\frac{B_T \mathbb{T}_0}{4\mathbb{S}_0} \right)^2 + \frac{4tol}{12\mathbb{S}_0 C_{PFE}} \right)^{1/2} \right)^{1/r}$$

Assuming that N_h grows as $\mathcal{O}(h^{-d})$ then

$$N_h(tol) \geq D_3 \left(-\frac{B_T \mathbb{T}_0}{2\mathbb{S}_0} + \left(\left(\frac{B_T \mathbb{T}_0}{4\mathbb{S}_0} \right)^2 + \frac{4tol}{12\mathbb{S}_0 C_{FE}} \right)^{1/2} \right)^{-d/r}$$

for some constant $D_3 > 0$.

(c) **Sparse Grid:** We seek $\|\hat{Q}_h(\mathbf{y}_s, \mathbf{0}) - \mathcal{S}_w^{m,g} \hat{Q}_h(\mathbf{y}_s, \mathbf{0})\|_{L^2_\rho(\Gamma)} \leq \frac{tol}{3C_{PSG}}$. This is satisfied if $\|e_0\|_{L^2_\rho(\Gamma_s; H^1_0(U))} \leq \frac{tol}{6a_{max} \mathbb{F}_{max}^d \mathbb{F}_{min}^{-2} C_{PSG}}$ and

$$\|e_n\|_{L^2_\rho(\Gamma_s; L^2(U))} \leq \frac{tol}{6B_T C_{PSG}}$$

for $n = 1, \dots, N_f$. Following the same strategy as in [18] (equation (3.39)), to simplify the bound (29) choose $\delta^* = (e \log(2) - 1)/\tilde{C}_2(\sigma)$. Thus $\|\hat{Q}_h(\mathbf{y}) - \mathcal{S}_w^{m,g} \hat{Q}_h(\mathbf{y})\|_{L^2_\rho(\Gamma)} \leq \frac{tol}{3C_{PSG}}$ if

$$\eta_0(tol) \geq \left(\frac{6a_{max} \mathbb{F}_{max}^d \mathbb{F}_{min}^{-2} C_{PSG} C_F F^{N_s} \exp(\sigma(\beta))}{tol} \right)^{\frac{1+\log(2N_s)}{\sigma}}$$

for a sufficiently large N_s , where $C_F := \frac{C_1(\sigma, \delta^*, \tilde{M})}{|1 - C_1(\sigma, \delta^*, \tilde{M})|}$, and $F := \max\{1, C_1(\sigma, \delta^*, \tilde{M})\}$. Similarly, for a sufficiently large N_s we have that

$$\eta_n(tol) \geq C \left(\frac{6B_T C_{PSG} C_F F^{N_s} \exp(\sigma(\beta))}{tol} \right)^{\frac{1+\log(2N_s)}{\sigma}}$$

for $n = 1, \dots, N_f$.

Combining (a), (b) and (c) into equations (30) and (31) we obtain the total work $W_{Total}^{mean}(tol)$ and $W_{Total}^{var}(tol)$ as a function of a given user error tolerance tol .

8. NUMERICAL RESULTS

In this section we test the hybrid collocation-perturbation method on an elliptic PDE with stochastic deformation of the unit square domain i.e. $U = (0, 1) \times (0, 1)$. The deformation map $F : U \rightarrow \mathcal{D}(\omega)$ is given by

$$\begin{aligned} F(x_1, x_2) &= (x_1, (x_2 - 0.5)(e(x_1, \omega)) + 0.5) & \text{if } x_2 > 0.5 \\ F(x_1, x_2) &= (x_1, x_2) & \text{if } 0 \leq x_2 \leq 0.5. \end{aligned}$$

According to this map only the upper half of the square is deformed but the lower half is left unchanged. The cartoon example of the deformation on the unit square U is shown in Figure 3.

The Dirichlet boundary conditions are set according to the following rule:

$$u(x_1, x_2)|_{\partial D(\omega)} = \begin{cases} \vartheta(x_1) & \text{upper border} \\ 0 & \text{otherwise} \end{cases}$$

where $\vartheta(x_1) := \exp(\frac{-1}{1-4(x_1-0.5)^2})$. Note that the boundary condition on the upper border does not change even after the stochastic perturbation.

For the stochastic model $e(x_1, \omega)$ we use a variant of the Karhunen Loève expansion of an exponential oscillating kernel that are encountered in optical problems [15]. This model is given by

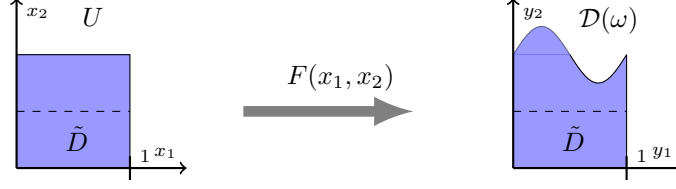


FIGURE 3. Stochastic deformation of unit square U according to the rule given by $F : U \rightarrow \mathcal{D}(\omega)$. The region \tilde{D} is not deformed and given by $(0, 1) \times (0, 0.5)$.

$$e_s(\omega, x_1) := 1 + cY_1(\omega) \left(\frac{\sqrt{\pi}L}{2} \right)^{1/2} + c \sum_{n=2}^{N_s} \sqrt{\mu_n} \varphi_n(x_1) Y_n(\omega);$$

$$e_f(\omega, x_1) := c \sum_{n=1}^{N_f} \sqrt{\mu_{n+N_s}} \varphi_n(x_1) Y_n(\omega)$$

with decay $\sqrt{\mu_n} := \frac{(\sqrt{\pi}L)^{1/2}}{n^k}$, $n \in \mathbb{N}$, $k \in \mathbb{R}^+$ and

$$\varphi_n(x_1) := \frac{\sin\left(\frac{n\pi x_1}{2L_P}\right) - \cos\left(\frac{n\pi x_1}{2L_P}\right) + \cosh(x_1) + \sinh(x_1)}{n}.$$

It is assumed that $\{Y_n\}_{n=1}^N$ are independent uniform distributed in $(-\sqrt{3}, \sqrt{3})$, thus $\mathbb{E}[Y_n] = 0$, $\mathbb{E}[Y_n Y_m] = \delta[n - m]$ for $n, m = 1 \dots N$ where $\delta[\cdot]$ is the Kronecker delta function.

It can be shown that for $n > 1$ we have that

$$B_n = \begin{bmatrix} 0 & 0 \\ c(x_2 - 0.5)\partial_{x_1}\varphi_n(x_1) & 0 \end{bmatrix}.$$

This implies that $\sup_{x \in U} \sigma_{\max}(B_l(x))$ is bounded by a constant. Thus for $k = 1$ we obtain linear decay on the gradient of the deformation. In Figure 4 two mesh examples of the domain U and a particular realization of $\mathcal{D}(\omega)$ with the model $e(x_1, \omega)$ are shown with the Dirichlet boundary conditions.

The QoI is defined on the bottom half of the reference domain (\tilde{D}), which is not deformed, as

$$Q(\hat{u}) := \int_{(0,1)} \int_{(0,1/2)} \vartheta(x_1) \vartheta(2x_2) \hat{u}(\omega, x_1, x_2) dx_1 dx_2.$$

In addition, we have the following:

- (i) $a(x) = 1$ for all $x \in U$, $L = 1/2$, $L_P = 1$, $N = 15$.
- (ii) The domain is discretized with a 2049×2049 triangular mesh.
- (iii) $\mathbb{E}[Q_h]$, $\mathbb{E}[Q_h^2]$, and $\sum_{i=1}^{N_f} \mu_{f,i} \mathbb{E}[\int_U \tilde{\alpha}_{i,h}]^2$ are computed with the Clenshaw-Curtis isotropic sparse grid from the *Sparse Grids Matlab Kit* [22, 2].
- (iv) The reference solutions $\text{var}[Q_h(u_{ref})]$ and $\mathbb{E}[Q_h(u_{ref})]$ are computed with a dimension adaptive sparse grid (*Sparse Grid Toolbox V5.1* [8, 14, 13]) with Chebyshev-Gauss-Lobatto abscissas for $N = 15$ dimensions.
- (v) The QoI is normalized by the reference solution $Q(U)$.
- (vi) The reference computed mean value is 1.054 and variance is 0.1122 (0.3349 std) for $c = 1/15$ and cubic decay ($k = 3$).

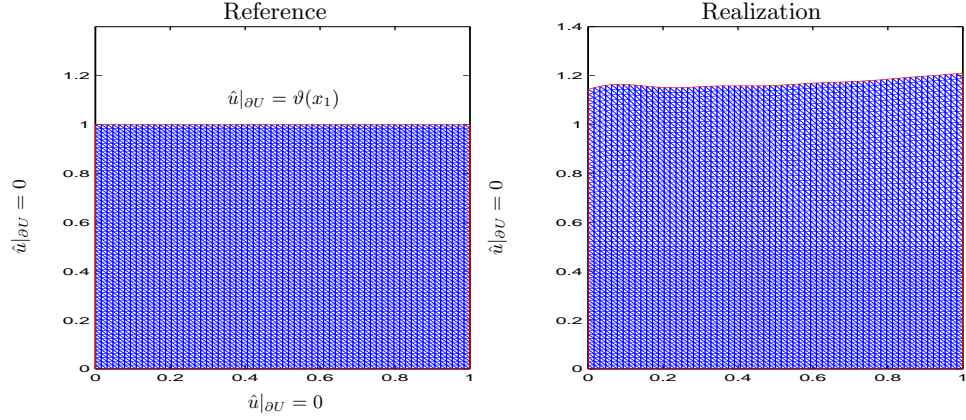


FIGURE 4. Stochastic deformation of a square domain. (left) Reference square domain with Dirichlet boundary conditions. (right) Vertical deformation from stochastic model.

Remark 12. *The correction variance term is computed on the fixed reference domain U as described by Problem 1 instead of the perturbed domain. The pure collocation approach (without the variance correction) and reference solution are also computed on U . Numerical experiments confirm that computing the pure collocation approach on U , as described by Problem 1, or the perturbed domain $\mathcal{D}(\omega)$ lead to the same answer up to the finite element error. This is consistent with the theory.*

For the first numerical example we assume that we have cubic decay of the deformation i.e. the gradient terms $\sqrt{\mu_n} \sup_{x \in U} \|B_n(x)\|$ decay as n^{-3} . The domain is formed from a 2049×2049 triangular mesh. The reference domain is computed with 30,000 knots (dimension adaptive sparse grid). In Figure 5(a) we show the results for the hybrid collocation-perturbation method for $c = 1/15$, $k = 3$ (cubic decay), $N_s = 2, 3, 4$ dimensions and compare them to the reference solution. For the collocation method the level of accuracy is set to $w = 5$. For the variance correction we use $w = 3$ since there is no benefit to increase w as the sparse grid error is smaller than the perturbation error. The observed computational cost for computing the variance correction is about 10% of the collocation method.

In Figure 5(b) we compare the results between the pure collocation [5] and hybrid collocation-perturbation method. Notice the hybrid collocation-perturbation shows a marked improvement in accuracy over the pure collocation approach.

Remark 13. *Note that the number of knots of the sparse grid are computed equally for the pure collocation and variance correction for this case. However, in practice the number of sparse grid knots needed for the variance correction are small compared to the pure collocation approach. These are due to the fact that the variance correction is scaled by the coefficients μ_n^f for $n = 1, \dots, N_f$.*

In Figure 6(a) and (b) the variance error decay plots for $k = 3$ (cubic) and $k = 4$ (quartic) are shown for the collocation (dashed line) and hybrid methods (solid line). The reference solutions are computed with a dimension adaptive sparse grid with 30,000 knots for the cubic case and 10,000 knots for the quartic case. The

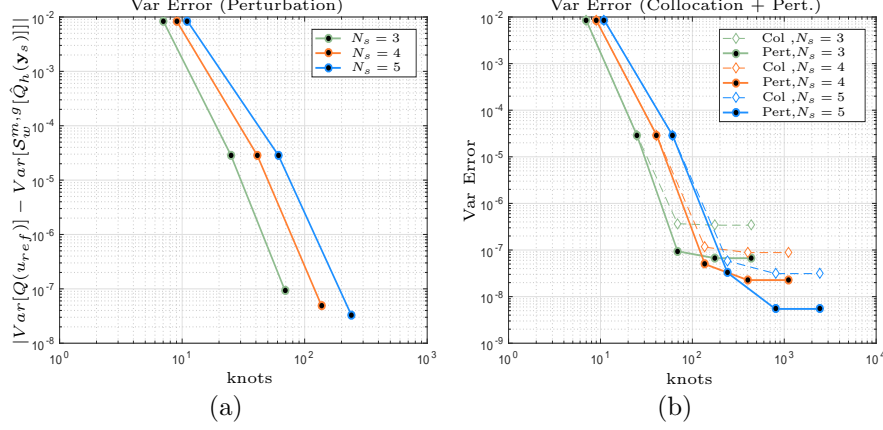


FIGURE 5. Hybrid Collocation-Perturbation results with $k = 3$ (cubic decay) and $c = 1/15$. (a) Variance error for the hybrid collocation-perturbation method with respect to the number of collocation samples with an isotropic sparse grid. The maximum level is set to $w = 3$. (b) Comparison between the pure collocation (Col) and the hybrid collocation-perturbation (Pert) approaches. As we observe the error decays significantly with the addition of the variance correction. However, the graphs saturate once the perturbation/truncation error is reached. Note that the number of knots of the sparse grid are computed up to $w = 5$ for the pure collocation method. For the variance correction the sparse grid level is set to $w = 3$ since at this point the error is smaller than the perturbation error and there is no benefit to increasing w . The sparse grid knots needed for the variance correction are almost negligible compared to the pure collocation.

collocation and hybrid estimates are computed with an isotropic sparse grid with Clenshaw-Curtis abscissas.

It is observed that the error for the hybrid collocation-perturbation method decays faster, as the dimensions are increased, compared to the pure collocation method. Moreover, as the dimensions are increased the accuracy gain of the perturbation method accelerates significantly (c.f. Figure 6(b)). The accuracy improves from one order of magnitude to 23 times improvement. We expect the accuracy to further accelerate as we increase w . However, we are limited in computational resources to compute larger mesh sizes.

9. CONCLUSIONS

In this paper we propose a new hybrid collocation perturbation scheme to computing the statistics of the QoI with respect to random domain deformations that are split into large and small deviations. The large deviations are approximated with a stochastic collocation scheme. In contrast, the small deviations components of the QoI are approximated with a perturbation approach.

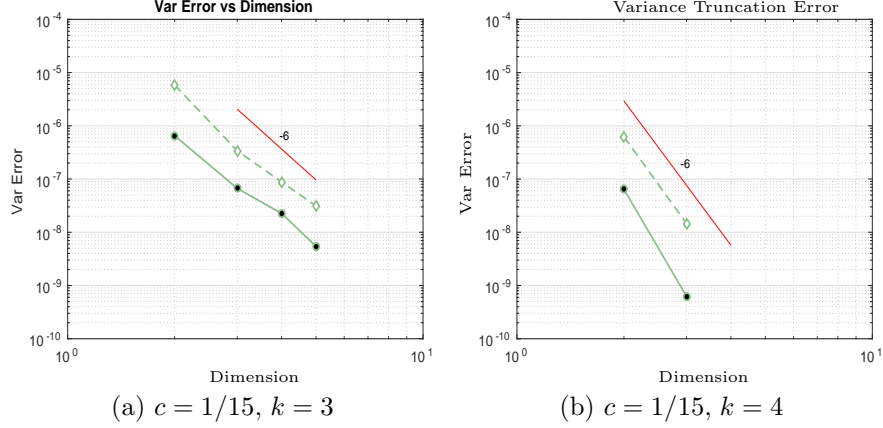


FIGURE 6. Truncation error with respect to the number of dimensions and different decay rates. (a) Variance error for the pure collocation (dashed line) and hybrid collocation-perturbation (solid line) methods for $c = 1/15$ and $k = 3$. (b) Variance error ratio between the collocation and hybrid methods for $c = 1/15$ and $k = 4$. Notice that the accuracy of the hybrid collocation-perturbation significantly increases with dimensions.

We give a rigorous convergence analysis of the hybrid approach based on isotropic Smolyak grids for the approximation of an elliptic PDE defined on a random domain.

We show that for a linear elliptic partial differential equation with a random domain the variance correction term can be analytically extended to a well defined region Θ_{β, N_s} embedded in \mathbb{C}^{N_s} with respect to the random variables. This analysis leads to a provable subexponential convergence rate of the QoI computed with an isotropic Clenshaw-Curtis sparse grid. We show that the size of this region, and the rate of convergence, is directly related to the decay of the gradient of the stochastic deformation.

This approach is well suited for a moderate to a large number of stochastic variables. Moreover we can easily extend this approach to anisotropic sparse grids [17] to further increase the efficiency of our approach with respect to the number of dimensions.

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